CaRIne Crystallography 3.1

for Microsoft Windows

© 1989-1998 C. Boudias & D. Monceau

User's Guide

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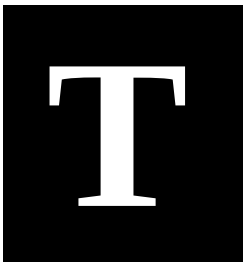

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INTRODUCTION I

Basic crystallography will often appear as an obvious subject for... crystallographers! But every teacher had seen some students fighting with 3D representations and having troubles to understand the meaning of a stereographic projection from a drawing on the blackboard. The teacher will often have troubles to teach what seems to be a geometrical evidence.

The first purpose of CaRIne was to help the non-specialist to visualize 3D-structures (cells, planes, directions...). The "computer tool" was chosen because of its capacities to access to the third dimension through rotations. It was also preferred to ball & stick models because of its versatility and interactive qualities.

In June 89, CaRIne was born and able to draw every structures, simple ones and complex ones, thanks to a good mathematical background. The early success of CaRIne in France brought to the authors many comments and suggestions, and the software evoluated from versions 1.0 to version 2.5.

In 93, the idea had come to extend the software to other representations, using the new possibilities of computers interactivity and ease to use. Version 3.0 was conceived in September and one year later it began to be distributed for Mac and in French only.

This new local success has encouraged the authors to bring the software to the more popular Microsoft Windows environment. Since 89 CaRIne has evoluated to become an useful tool for teaching and now also for edition and research. With this new English translation, we hope that our work will help numerous persons all around the world in their everyday work.

Waiting for your feedback,

the authors.

Note :

We don't think it is necessary to read all the user manual in details before to start. But, after a first contact with the software, we encouraged the user to read chapters 1 and introductions of chapters 6, 7 and 8, which explain the "philosophy" of this work. Then, you can exercise with chapter 9. To get some help on a precise function you will reference to chapter 2 for the real lattice, 6 for the stereographic projection, 7 for the X-Rays Diffraction, 8 for the reciprocal lattice. You can also have a fast general look to the manual to know what it is possible to do, and you will find a lot of pictures !

It is now time to wish you "bon voyage".

Many thanks to :

Denis Ansel, Sam et Jean Blachère, Bernadette Baroux, Sophie et Pascal Bartek, Gérard Béranger, Dagmara Berztiss, Nicolas Boëns, Guillaume Boucher, Sandrine Boudias, Bernadette et Bernard Boudias, Yves Breton, Sophie Bruges, Philippe Buffat, Françoise Cabané, Daniel Cabrol, Rémi Capet, Kay Chhor, Michel Clavel, Alain Dautant, Frank Elstner, Philippe Buffat, Yves Franchot, Yvan Guillot, Alain Hewat, Julitte Huez, Timothy Klemmer, Kate Krenell, Alina Klimczyk, Jean Laugier, K'TO Manning, Claudine et Bernard Monceau, Claude Monty, Georgette Petot-Ervas, Claude Petot, Jean Philibert, Claude Pommier, Laurence Pouchenot, Jean-Pierre Rabine, Bill Soffa, Mr T...

CHAPTER 0
Installation Procedure

0

This Chapter is dedicated to the installation procedure of CaRIne.

0.1 Before Installation

Before installing CaRIne 3.1, you should check the following points :

- Have a look at the " *readme.txt*" file, located on the install disk or CD-ROM. This file contains information which couldn't be written in time on the user manual. It can be opened with any word processor (Notepad or WordPad for example);
- Make a copy of your installation floppy;
- Fill in and send the registration card, in order to get full technical assistance and to be informed of the new versions coming out at the best price.

System Requirements :

CaRIne 3.1 requires the following minimum configuration :

- An IBM Personal Computer, or 100 percent compatible, running Microsoft Windows 95/NT4.0 or higher.
- An 486 or higher processor.
- Height megabytes of available memory (8MB RAM).
- A 1.44-MB, 3.5-inch disk drive or CD-ROM.
- 20 free MB on the hard disk drive.

0.2 Installation

0.2.1 Install procedure

The Setup program provided by CaRIne Crystallography performs all tasks necessary for installing the CaRIne components. You can install everything at once or install just a subset and upgrade it later with additional libraries, samples, help files, or other components.

To run Setup :

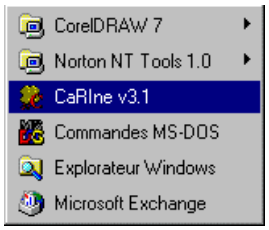
1. Place Disk 1 in drive A (or B...) or CD-ROM.

2. From the control panel select Add/Remove programs menu and type A:\Setup in the command line box.

3. Install prompts you with a dialog box that describes the program and lets you continue or exit.

4. Follow the installation instructions.

When the installation procedure is ended, Setup add CaRIne 3.1 in the Start Menu :



To run the CaRIne 3.1 program, select it on the Start menu.

To select the language of CaRIne, choose *File|Options*. It is possible to switch between French and English while the program is running.

0.2.2 Install on a network

When following the install procedure (given in 0.2.1), the libraries will be automatically placed in the same directory as the CaRIne v3.1 program.
As a consequence, users without writing rights on the network server disks will not be able to save their own files in the default directories.
To solve this problem, a new default folder has been created : *Personal directory* which needs to be setup by every network user (see 0.3.3).

0.2.3 File Compatibilities

Note : CaRIne v3.1 is able to read your 3.0 version files, but version 3.0 will not read v3.1 files ! If you really need to go back from v3.1 to v3.0, you may use the ASCII files (ACE and ACR) which are fully compatibles (even with the Mac version).

As a 32 bits windows application, CaRIne v3.1 allows 255 character file names.

Icons have been changed in order to differentiate version 3.0 and 3.1 cells and crystals files.

: for cell files (extension CEL)

: for crystal files (extension CRY)

0.3 Files and directories

0.3.1 Data Base directories

When following the install procedure (given in 0.2.1), the libraries will be automatically placed in the same directory as the CaRIne 3.1 program. In order to have a quick access to these files, CaRIne proposes to associate them with directories. To set all the associated directories, select the function *File* | *Options*.

0.3.2 Import-Export directory

A new default directory has been added in version 3.1 : «Import-Export». It concerns all the text files created by CaRIne (angle list, X-Ray diffraction list, ...). Use the *File*|*Options* function to set this directory.

0.3.3 Personal directory

In case you need to load/save your files all in the same directory, CaRIne offers you the possibility to define a personal directory. This function is especially useful in case of a network utilization. To select your personal directory call the *File/Option* function, define your folder and check the box "use the personal directory"

0.3.4 How to stay in the current directory

When loading or saving several files, it is now possible to stay in the same directory. To do so, press on the *Alt* key when loading or saving a file (*File*|*Load* or *Save*).

0.3.5 Drag and drop CEL and CRY files

In order to facilitate the loading and saving of CEL and CRY files, it is now possible to select these files from the Explorer and to «drag and drop» them onto the CaRIne application.

CHAPTER 1
CaRIne and the crystallography 1

This chapter describes how different crystallographic concepts are approached and interpreted by the software.

1.1 Notions of unit cell, lattice, lattice points, motif, crystal,...

Lattice / Lattice points :

The lattice is classically defined as a group of points organised in space in such a way that each point has the same environment.

Motif :

The motif is the minimal unit which is repeated in the lattice.

Unit cell :

The unit cell is the volume defined by the lattice vectors **a**, **b** and **c**. It is the minimal unit of volume which allows the construction of the total volume by unit cell juxtaposition (lattice translations).

Crystal :

CaRIne software interprets "crystals" as being all information which allows the construction of a complete representation.
The following table clarifies this point by describing what is contained in each object corresponding to crystallographic concepts :

Motif	• the list of non-equivalent atoms
Unit cell	• the list of all atoms found in the volume (**a**,**b**,**c**) • the cell parameters (which define the system)
Crystal	• the unit cell as above • the number of cells following the directions of **a**, **b** and **c** • all modifications applied to the atoms (displacement, substitution, vacancy, interstitial,…) leading to a non-respect of lattice translations.

Table 1.1 : Motif, Unit cell and Crystal

The following paragraph explains how CaRIne passes from one object to another.

1.2 Crystalline systems, Bravais' lattices, Space Groups

When cell parameters a, b, c, α, β, γ, are set, one of the **7 crystalline systems** is selected, which appears in the status bar, at the bottom of the window.

The choice of system can also be made by selecting a **Bravais' Lattice** . In which case the choice of system from the *Cell* Menu is followed by the choice of mode from the corresponding sub-menu (primitive, body-centred, base centred, face-centred).

CaRIne then opens a dialogue-box which allows the modification of the cell parameters (respecting the system) and a sphere is assigned to each point of the lattice. Obviously this sphere can be considered as an atom, and assigned a chemical symbol using Mendeleev's Periodic Table, which is available. However, this is not required, the spheres can also be assimilated to simple lattice points.

At this point, it would be preferable to be able to substitute a motif at each lattice point, and this function will be developed in a future version of CaRIne in which the lattice points and the atoms will be clearly distinguished. At the moment, this substitution can be made by using space groups. The choice of a group leads to a dialogue-box where the position of non-equivalent sites are entered. This defines a motif which will be repeated according to the group's elements of symmetry. There is therefore no obligation to place an atom at 0,0,0, for example.

e.g. : It is possible to choose the group 225 (Fm3m) and to enter a one-atom motif, placed at 1/2,0,0. The face centred cubic lattice is present but shifted from the origin.

The **space group** is the combination of all the possible transformations of symmetry in a crystalline structure. The space group characterises the symmetry of a crystalline structure in the same way that a **point group** characterises the symmetry of the exterior form of the crystal and the symmetry of its macroscopic properties. There are 32 point groups of symmetry (32 crystalline classes).

Each point group corresponds to several space groups. From the space group, the point group is obtained by eliminating all the translations. On the other hand, space groups can be deduced from the point groups. In order to do this, an examination of all the possible combinations between the symmetry elements of the point group and the translations of the type of lattice allowed by the point group is necessary.

230 space groups can be obtained. Each is a group in the mathematical sense of the word.

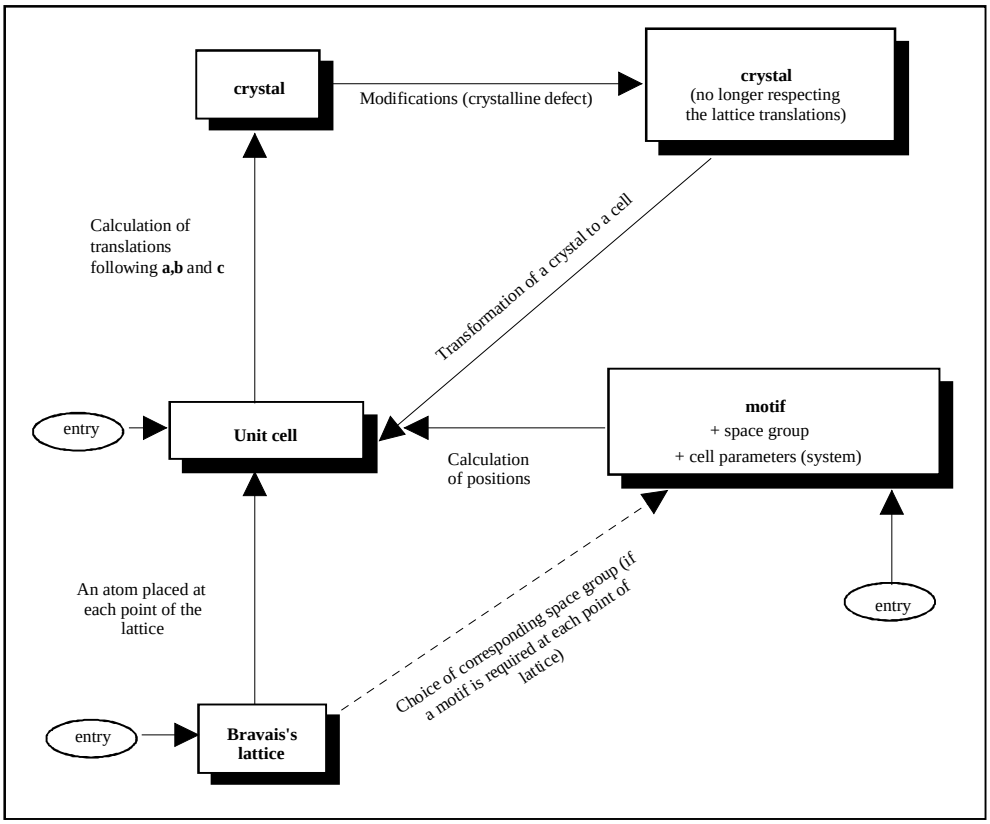


Fig 1.2 : Concept of creation of Motifs, Cells, Lattices and Crystals

1.3 Indexes of directions and planes

- To locate a crystallographic direction $\mathbf{d_{uvw}}$ or a row of atoms, the indi ces u, v and w are used. They are defined as follows:

  $\mathbf{d_{uvw}} = u.\mathbf{a} + v.\mathbf{b} + w.\mathbf{c}$
  where **a**, **b** et **c** are vectors of the unit cell and u, v, w are positive integers.

- For the planes, Mi ller's indi ces are used. For the family of planes {hkl}, the first plane inter sects the axes xx', yy', zz' at a/h, b/k and c/l when a, b and c are cell parameters.

- Conversion 3 ⇨ 4 indices (hexagonal system):

  $\mathbf{d_{uvw}} \Rightarrow \mathbf{d_{UVTW}}$ with
  $U = \frac{1}{3} \cdot (2 \cdot u - v),\ V = \frac{1}{3}(2 \cdot v - u),\ T = -(U + V)$ et $W = w$

  $\mathbf{d_{hkl}} \Rightarrow \mathbf{d_{HKTL}}$ with $H = h,\ K = k,\ T = -h - l$ et $L = l$

1.4 Use of CaRIne in 2D

In order to introduce the concept of punctual defects or elements of symmetry easily, a teacher may wish to work in two dimensions (2D). This is possible with CaRIne. The procedure is as following :

1 - define the parameters of the 2D cell : a, b and γ

2 - define the cell, with the atomic coordinate z placed at 0

3 - project in the direction perpendicular to the plane (001)

4 - Extend the lattice following **a**, **b** and **c**, with the required values of na and nc and especially **nc=0**

To carry out this sequence, see the description of the necessary functions in chapter two.

The second way to proceed is to work in a plane (hkl) (see the function : Selection of a plane (hkl), chap. .2). Once the plane has been selected, project perpendicularly to this plane, selecting only the atoms of the plane (hkl) in the graphic options (see chapter 4, command "**Graphics**").

1.5 Defects in crystals

The following table presents the functions made available by CaRIne, in order to represent crystalline defects.

Defect dimension	Kind of defect	Functions to use
dimension = 0	substitutionnal atom	Menu ***Crystal***, modify atom, or Menu ***Cell***, creation
	vacancy	Menu ***Crystal***, vacancy
	relaxation (move atoms)	Menu ***Crystal***, modify atom
	interstitial atom	Menu ***Crystal***, add atom
	Frenkel and Schottky defects	Menu ***Crystal***, modify atom, or Menu ***Crystal***, add atom
dimension = 1	dislocations	Menu ***Crystal***, modify atom in orc to move the concerned atom one l one !
dimension = 2	twin boundary	Menu ***Special***, relation of epitaxy or Associated lattices :
	grains boundary	just to study the orientation relationships between crystals.
dimension = 3	precipitate	

Table 1.3 : Defects in crystals

CaRIne possesses all the necessary functions for the creation of point defects. Future versions will include tools aimed at facilitating the representation of dislocations.

1.6 Units employed

The units of the International System are used, except in the case of atomic radii and sizes linked to them, where the Angstrom is preferred to the nanometer. The Angstrom is a unit which is coherent with the International System (1 Å=10^{-10}m). Moreover, the unit is widely used in crystallography because it is close to an atomic diameter, and also because it appears in the tables of interplanar distances of the JCPDS (Joint Committee for Powder Diffraction Standards).

Physical Variable	Unit	Symbol	Remarks
atomic radius	Angstroms	Å	
reduced atomic coordinates	without unit		between 0 and 1
oxidation degree	without unit		
occupation factor	without unit		between 0 and 1
cell parameters: a, b and c	Angstroms	Å	same unit than the atomic radii
cell parameters: α, β, and γ	degrees	°	
spread of lattice: na, nb and nc	without unit		integers positivesor nil
crystallographic direction u,v,w	without unit		integers positives or nil
crystallographic plane h,k,l	without unit		integers positives or nil
"thickness" of a plane:ε	without unit		real between 0 and 0.5
distance between atoms	Angstroms	Å	same unit as a, b and c
atomic coordonnates in the cell reference frame**a,b,c**	without unit		real positive or nil
angles between directions and planes	degrees	°	
cell volume V	cubic Angstro	$Å^3$	unit consistent with a, b and c
cell density	without unit		real between 0 and 1
wave length of X-rays: λ	Angstroms	Å	XRD and interplanar distances list
interplanar distance d_{hkl}	Angstroms	Å	
sum of squared indices:Σind^2	without unit		interplanar distances list
Bragg angle: θ	degrees	°	interplanar distances list
structure factor: F_{hkl}	without unit		interplanar distances list
multiplicity: p	without unit		interplanar distances list, integer > 0
relative intensity of a peak: I%	without unit	0-100%	XRD and interplanar distances list
accelerating voltage: V	kilo-Volts	kV	identification of planes
electrons wave-length ē: λ	Angstroms	Å	identification of planes
camera length: L	centimetres	cm	identification of planes
camera constant: K		cm.Å	identification of planes
distances on diffraction patterns: r1 and r2	centimetres	cm.Å	identification of planes
zone axis	without unit		cf. uvw
Physical Variable	Unit	Symbol	Remarks
solid angle: S.A.%	without unit	0-100%	shells

number of atoms in a layer: nb	without unit		shells, integer positive or nil
temperature factor	squared Angstroms	$Å^2$	XRD, real between 0 and 20 (or more)
poles	without unit		stereographic projection , cf. hkl
traces	without unit		stereographic projection, cf. hkl
angles θ and ϕ	degrees	°	stereographic projection
links thickness	without unit		integer between 0 and 10 (or more)
size of shading zone	pixel		integer between 0 and 50 (or more)
intensity variation	percent	%	shading due to depht

Table 1.4 : Units employed

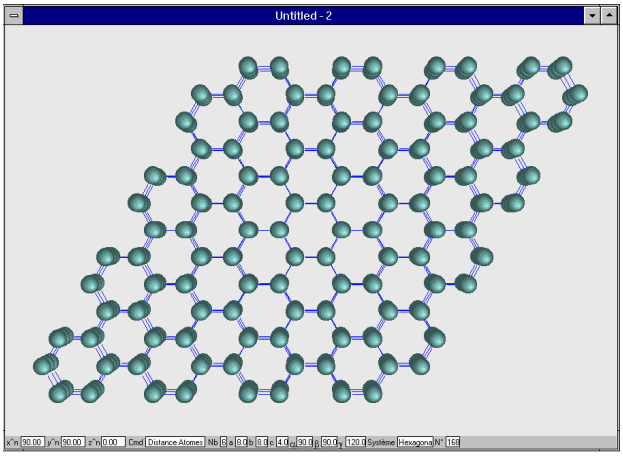
CHAPTER 2
General description of CaRIne

2

This chapter describes the different types of windows managed by CaRIne and the commands which are associated with them.

2.1 The different types of windows

The "Crystal" windows



F2.1 : The "Crystal" windows.

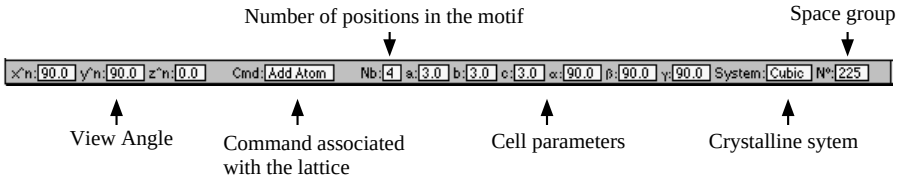
The "crystal" windows allow the visualisation of your crystal structures. Their size can be modified, the lattice is always centred in its window. The function associated with "real lattice" windows are described throughout this chapter. At the bottom of such a window, a status bar which gives the angle of view, the current command and the cell parameters,.... can be found.

The status bar

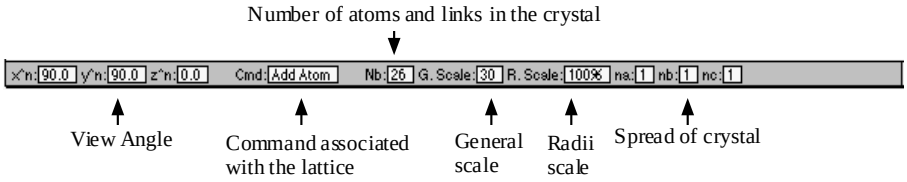
The status bar is composed of 4 sections. In order to change the sections, click on the status bar. Each section is composed of angles which define the angle of view and the command associated with the lattice at the time.

A command can be selected from a menu, using the mouse, the corresponding short key or by using the tool palettes. This command is shown in the status bar and remains active until another command has been selected.

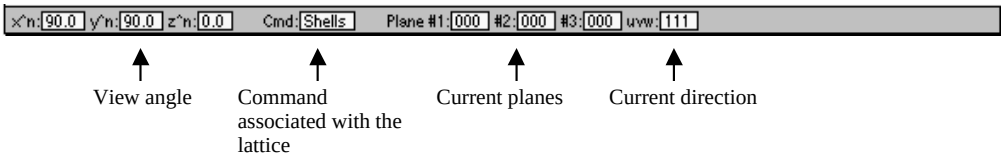
- Information on the cell :


Number of positions in the motif
Space group
x'n: 90.0 y'n: 90.0 z'n: 0.0 Cmd: Add Atom Nb: 4 a: 3.0 b: 3.0 c: 3.0 α: 90.0 β: 90.0 γ: 90.0 System: Cubic N°: 225
View Angle
Command associated with the lattice
Cell parameters
Crystalline sytem

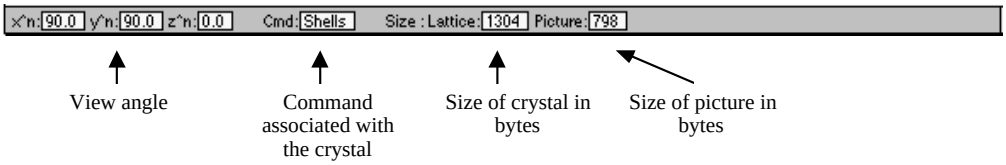
- Information on the crystal :


Number of atoms and links in the crystal
x'n: 90.0 y'n: 90.0 z'n: 0.0 Cmd: Add Atom Nb: 26 G. Scale: 30 R. Scale: 100% na: 1 nb: 1 nc: 1
View Angle
Command associated with the lattice
General scale
Radii scale
Spread of crystal

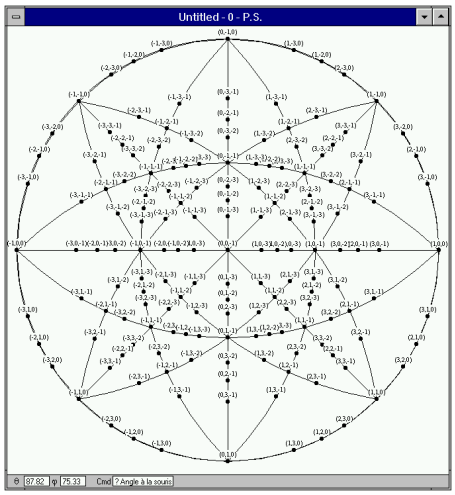
- Information on planes and direction :


x^n: 90.0 y^n: 90.0 z^n: 0.0 Cmd: Shells Plane #1: 000 #2: 000 #3: 000 uvw: 111
View angle
Command associated with the lattice
Current planes
Current direction

- Information on memory :


x^n: 90.0 y^n: 90.0 z^n: 0.0 Cmd: Shells Size : Lattice: 1304 Picture: 798
View angle
Command associated with the crystal
Size of crystal in bytes
Size of picture in bytes

The "Stereographic projection" windows

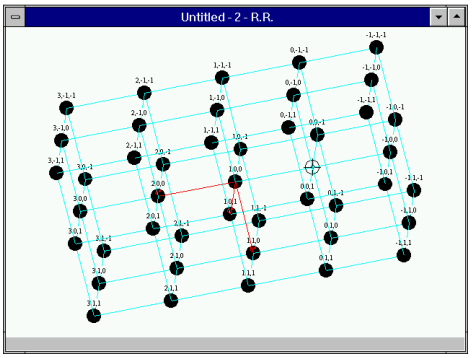


F2.2 : The "Stereographic projection" window.

The "Stereographic projection" windows enables the visualisation of the Stereographic projections corresponding to the active crystal window (see Chap. 6). The size of the stereographic projection automatically adapts itself to that of the window. There is only one window of this type for each crystal. The associated commands are situated in the *Special/Stereo. Proj.* Menu.

At the bottom of each "stereographic projection" window there is a status bar where the angles corresponding to the present position of the protractor and the associated command can be found.

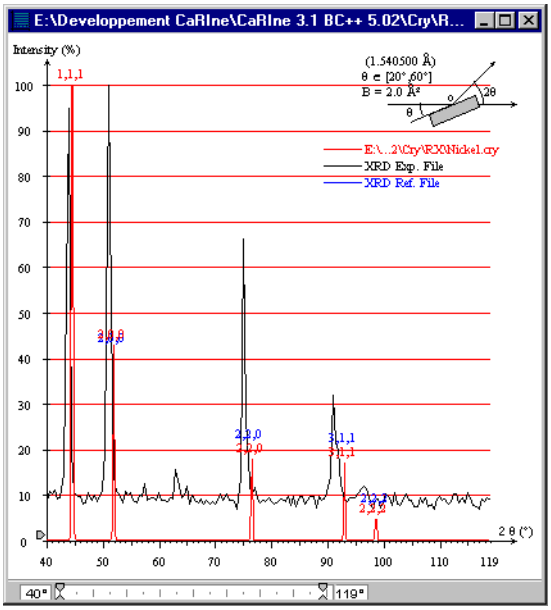
The "reciprocal lattice" windows



F2.3 : The "Reciprocal lattice" window.

The "reciprocal lattice" windows allow the visualisation of reciprocal lattices corresponding to the active real lattice (see Chap. 8). There is only one window of this type associated with each crystal. The appropriate commands are situated in the ***Special./Reciprocal Lattice*** Menu.
At the bottom of each "reciprocal lattice" window there is a status bar, where the current command can be found.

The "XRD" windows



F2.4 : The "XRD" window

The "XRD" windows allow the visualisation of the X-Ray diffraction diagram corresponding to the active real lattice. There is only one window of this type associated with each crystal. The appropriate commands can be found in the ***Special./XRD Powder*** Menu

The "Tool palettes" windows

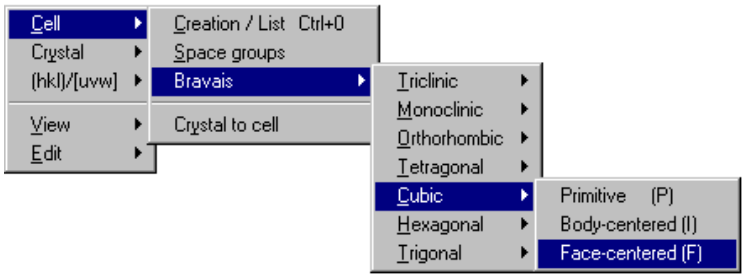
CaRIne has three "tool palettes" which allow rapid access to the functions of the Crystal, Special and View Menus. These are floating windows (they are always above the desktop of your computer) and can be hidden or activated with the help of the "**…tools**" functions from the *Windows* Menu.

In this manual, if an icon appears in front of a command (or a function) of a menu, access to it is available through one of the tool palettes.

Context menus

Every window possesses a specific context menu (crystal, stereographic projection, reciprocal lattice, XRD).

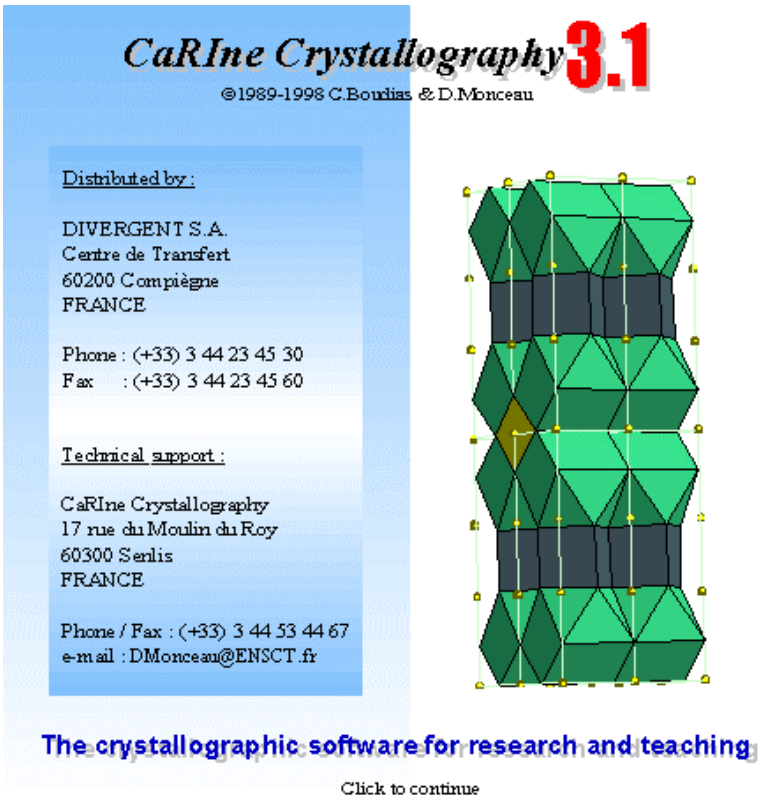
Those context Menus allow a fast access to the associated functions. To activate a context menu, simply click inside a window with the right mouse button.



Context menu of a crystal Window

About CaRIne...

This function allows you to find rapidly the addresses of both authors and distributor, as well as information concerning the copyrights.



F2.5 : About CaRIne.

2.3 *Files* Menu

The functions of the ***Files*** Menu permit the management of your document files. There are 3 sorts of files :

- Motif or Cells (CEL, MTF2, MTF*)
- Crystals (CRY, RES2, RES*)
- Pictures (WMF, PICT)

CaRIne allows several crystal files of the same unit cell to be saved. In order to differentiate these files, CaRIne automatically gives the extension ".cel" to the motif files and ".cry" to the crystal files (see Chap.3)

CaRIne also manages the importation and exportation of motifs and lattices from the ASCII files ("text" format).

New Ctrl-N

This command allows the creation of a new "crystal" window, a prop for the representation of a crystalline lattice. A new motif should be constructed (see Chap. 3) .

When a cell or a lattice is loaded from the data bases, a window is automatically created without having to use this "**New**" function.

Close Ctrl-F4

After confirmation, this command allows the closure of the current "crystal" window, as well as all other associated windows (stereographic projection, reciprocal lattice and XRD windows).

Open Cell Ctrl-O, Save Ctrl-S, Save As...

The first three commands of the *Files* Menu allow the saving, saving under another name, and loading of a file containing all the information relating to a motif (see Appendix A).

Open Crystal Ctrl-Shift-O, Save Ctrl-Shift-D, Save As...

The functions relating to the crystal files are similar to those of the motif files.

For CaRIne, a crystal (see Appendix A) is defined as being one or several unit cells, with modifications of links and atoms (substitutions, interstitials, vacancies, displacements…) and with polyhedrons. When a crystal is saved, the created file contains the motif which has allowed its construction, the modifications applied to it and all the information concerning the view (planes, directions, scales,…). Additionally, if the stereographic projection, the reciprocal lattice, or the diffraction diagram exist, they will also be saved.

Save Picture As...

The associated command allows the picture representing the crystal, the stereographic projection, the reciprocal lattice or the X-Ray diffraction diagrams to be saved, using the WMF format. The created files can be imported to all applications (word processing, picture softwares etc…) which accept this file format. Obviously, a function permitting the loading of such images doesn't exist because CaRIne deals with 3D structures, whereas these images are simple 2D projections.

Import

This sub-menu manages the importation of cells or crystals from ASCII files.

Cell Standard ASCII File

This function allows the importation of a cell from a "Cell Standard ASCII File" file format (see Appendix A). It can also be used to import cell or lattice description files (with space group) from another software. The function is equally used to visualise the results of other calculation programs (Molecular Dynamics, for example).

Cell *.MTF

This function allows the importation of a cell from an ASCII file created with CaRIne for DOS.

Cell CaRIne Macintosh

This function allows the importation of a cell from a file created with CaRIne 3.0 for Macintosh.

Crystal Standard ASCII File

This function allows the importation of a crystal from a "Crystal Standard ASCII File" file format (see Appendix A). It can also be used to import cell or lattice description files (with space group) from another software.

Crystal *.RES

This function allows the importation of a crystal from a ASCII file of CaRIne versions for DOS (files *.RES).

Export

This sub-menu manages the exportation of cells or crystals to ASCII files.

Cell Standard ASCII File

This function allows the exportation of a cell to a "Cell Standard ASCII" format file (see Appendix A). After possible transformations, this file could be imported to other software.

Crystal Standard ASCII File

This function allows the exportation of a cell to a "Crystal Standard ASCII" format file (see Appendix A). In this way, a list of all objects visualised on the screen and in particular, the real coordinates of all the atomic positions in an orthonormal frame can be obtained.

Standard ASCII File Prefs

This function allows the options necessary to export a crystal or unit cell to a standard ASCII file.

You have to choose the colours reference and you need to precise if you want to save the equivalent positions (see Appendix A).

F2.6 : Exportation parameters.

Print preview

This function allows to preview all drawings made by CaRIne.

Print setup...

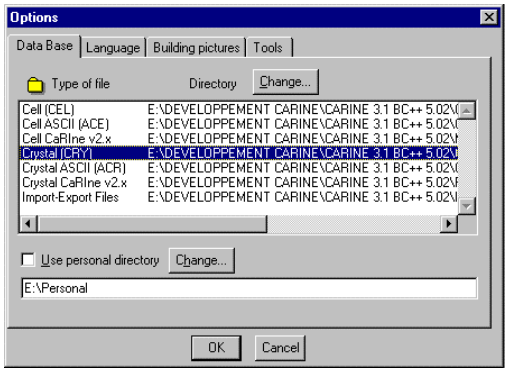
This function allows the page-setting of your documents.

Print... Ctrl-P

Real lattices, reciprocal lattices, X-Ray diffraction diagrams and stereographic projections can be printed (of course, the corresponding window should be activated).

Note : Change the value of **Radii** in the registry to set the radii of the stereographic projections when they are printed (see the description of the key : *HKEY_CURRENT_USER\Software\CaRIne\3.1\Stereographic projection* in Appendix B).

Options



This function allows you to select CaRIne's language, the default directories, the waiting bar during drawing processing, and the size of icons.

You have to restart CaRIne when you modify the size of icons.

Quit Alt-F4

This command allows you to quit CaRIne.

2.4 *Edit* Menu

The functions of this menu allow the utilisation of the copy/paste functions.

Undo/Redo Ctrl-Z

This function allows the user to undo or redo the last command if permitted.

Copy Ctrl-C

All the images formed by CaRIne (crystals, reciprocal lattices, stereographic projections and X-Ray diffraction diagrams) can be copied, and pasted into the clipboard, a document from your word processor or your drawing software.

A drawing software (such as CorelDraw * or Draw * for example) allows a picture to be modified, captions, frames and remarks to be added and even the displacement of atoms.

Using a picture software also allows real and reciprocal lattices, stereographic projections and X-Ray diffraction diagram to be assembled in the same figure.

2.5 *Cells* Menu

The following functions allow you to define your own motifs or unit cells.

Creation/List Ctrl-0

This function allows a new lattice to be created or all the positions of a unit cell to be listed (see Chap. 3 - Creation of a new unit cell).

Triclinic, Monoclinic, Orthorhombic, Trigonal, Hexagonal, Tetragonal, Cubic

These functions allow the crystalline system, as well as the type of lattice to be chosen. They permit access to the 14 Bravais' Lattices. The choice of type depends on the system selected (see Chap.3 - Use of Bravais' Lattices).

Space groups

Construction of a particular cell from a space group (see Chap. 3 - Construction of new motif, use of space groups).

Crystal to Cell

This function allows the current crystal to be transformed into a single unit cell.
In order to comply with lattice translations, only atoms with coordinates comply with the relations :

- $0 \leq x < na*a$
- $0 \leq y < nb*b$
- $0 \leq z < nc*c$

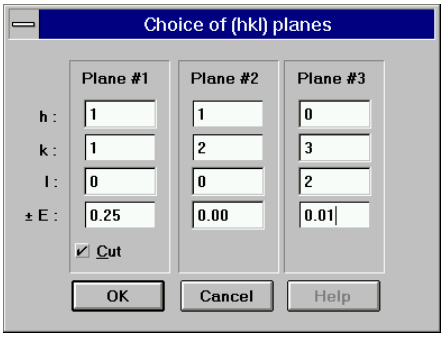
are accounted for (na, nb and nc are the number of cells following **a**, **b** and **c**).

2.6 *(hkl)/[uvw]* Menu

The functions which allow the visualisation and selection of planes and directions, in addition to the projections based on crystallographic indexes, are grouped together in this menu.

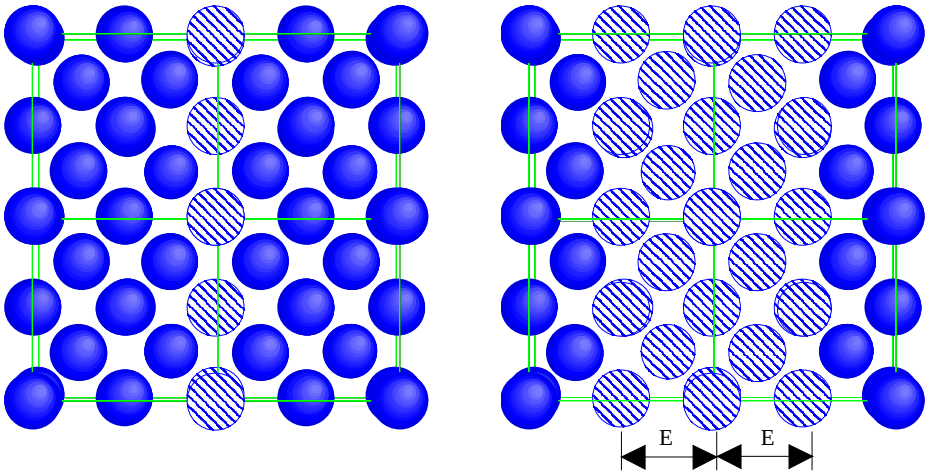
Choice of (hkl) planes Ctrl-H

It is possible to visualise three planes simultaneously. For each plane, the values h, k and l of the Miller indexes should be entered. Zero should be given as the value for h, k and l if no particular plane is required. The atoms contained in a plane are filled by a pattern corresponding to the number of the chosen plane (see table T2.11).



F2.7 : Miller's indexes entries.

E represents the "thickness" of a plane, and allows the visualisation of the atoms situated at a distance which is inferior to the value of "E" from the plane. This value should be between 0 and 0.5, as it is demonstrated in the following example which shows the plane (100) in a diamond lattice (na=2, nb=2, nc=1) :



(a) *E = 0*

(b) *E = 0.5*

F2.8 : Different values of E for the (100) plane in 4 diamond cells.

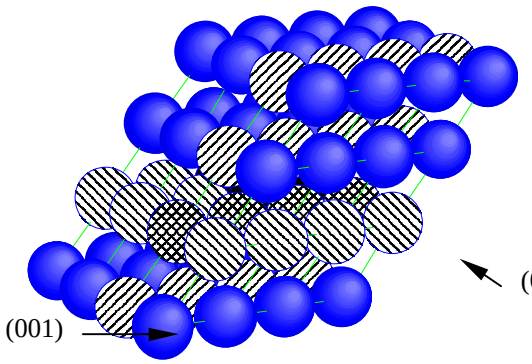
The exact definition of E is given by the following equation :

the atom with coordinates (x,y,z) in the frame (**a**,**b**,**c**) belongs to the plane (hkl) if, and only if :

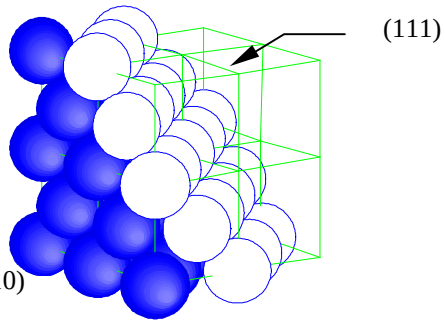
$$|h(x-t_a) + k*(y-t_b) + l*(z-t_c)-1+0.5*(|h|+|k|+|l| -h-k -l)| \leq (|h|+|k|+|l|)*E$$

where the vertical bars represent the absolute values, (t_a, t_b, t_c) the vector translation (expressed in the reference frame (**a**,**b**,**c**)) between the displayed plane and the plane with the same indices closest to the origin.

The crystal can be cut by the plane n°1 by ticking the check box ☒ **cut**. It is possible to modify the colour of the atoms belonging to the same plane (see "**Modify Atom** " function, Menu ***Crystal***), and in this way to show, for example, the stacking ABC of the cubic-centred faces (see Chap.9 E.g. 2).



F2.9 : Planes (001) and (010) in a triclinic lattice.



F2.10 : FCC cut by the plane (111).

If an atom belongs to the plane(s)	It appears as :
1	
2	
3	
1 et 2	
1 et 3	
2 et 3	
1, 2 et 3	

T2.11 : Filling motifs of atoms belonging to particular planes.

Translations ± of a plane Ctrl-T, Ctrl-B

These functions allow the translation of planes. In this way different successive representations of planes can be visualised (see Chap.4 *The translation of planes* , see also the e.g. of Chap.9 : Stacking ABCABC in FCC and ABAB in HCP).

Projection ⊥ to a plane Ctrl-K

This function allows the lattice to be projected following the normal of plane n°1 (see "**Choice of (hkl) planes**" function) if this is different from the plane (0,0,0). This projection is the function which should be used in order to find out about the structure and density of a particular plane. In this case, ask for the plane alone and remove the frame and the perspective effect (see ***View*** Menu).

If a stereographic projection window is opened, the corresponding pole will be placed in the centre of the projection.

? (hkl) with mouse

It is possible to obtain the Miller indices h, k and l of a particular plane by clicking on 3 non-aligned atoms. If the atoms are aligned, CaRIne attributes zero to each indice. This function is a quick, interactive and easy way to identify planes.

The indices h, k and l found in this way are attributed to the plane n°1, this function can be followed by "**Projection ⊥ to a plane**".

Choice of [uvw] direction Ctrl-U

This function opens a dialogue box which allows the indices u, v and w of a particular direction to be entered. This direction can be represented by a

vector (***View*** Menu). This is the current direction used by the following functions, and appears in the 3 rd status bar (see page 2-3).

Projection // to [uvw] Ctrl-J

This command creates a projection following the current direction. This direction is determined by the **"Choice of [uvw] direction"** or **"? [uvw] with mouse"** functions.

To obtain a real projection, the perspective effect must be removed (see "**Graphics**" function of the ***View*** Menu).

? [uvw] with mouse Ctrl-Y

It is possible to obtain the u, v and w indices of a direction by clicking on two atoms. The direction obtained in this way becomes the current direction and can be used to create a projection. This is a quick and interactive way of identifying directions or orientating a crystal.

2.7 Menu *Calcul.*

CaRIne is loaded with interactive tools which allow geometric measurements of crystallographic structures in 3D. By using the mouse, distances and angles are easily calculated without using usual trigonometric formulas.

Dist. Betw. 2 atoms

This function calculates the distance between two atoms chosen with the mouse. The coordinates of the atoms within the frame (**a**,**b**,**c**) are also obtained. This distance is given in Angstrom and is taken up by the function "**Multi-Link**" of the ***Crystal*** Menu (see page 2-42) and " **Spheres**" of the ***Specials*** Menu (see page 2-31).

Angle between directions, Angle between planes, Angle between plane and direction

These three functions calculate the angles between two directions, two planes, or a plane and a direction. The planes and the directions can be selected either by using the mouse or by entering their crystallographic indices. The angles are given in degrees.

> Attention : When asking for the angle between a plane and a direction using the mouse, the plane's atoms should be chosen before the two atoms of the direction.

Unit cell volume

This function calculates the volume V of the cell (in $Å^3$) :

$$V = \mathbf{a} \,.\, (\mathbf{b} \wedge \mathbf{c})$$

where $\wedge$ designates the vectorial product and **.** the scalar product.

Unit cell density

This function calculates the cell density :

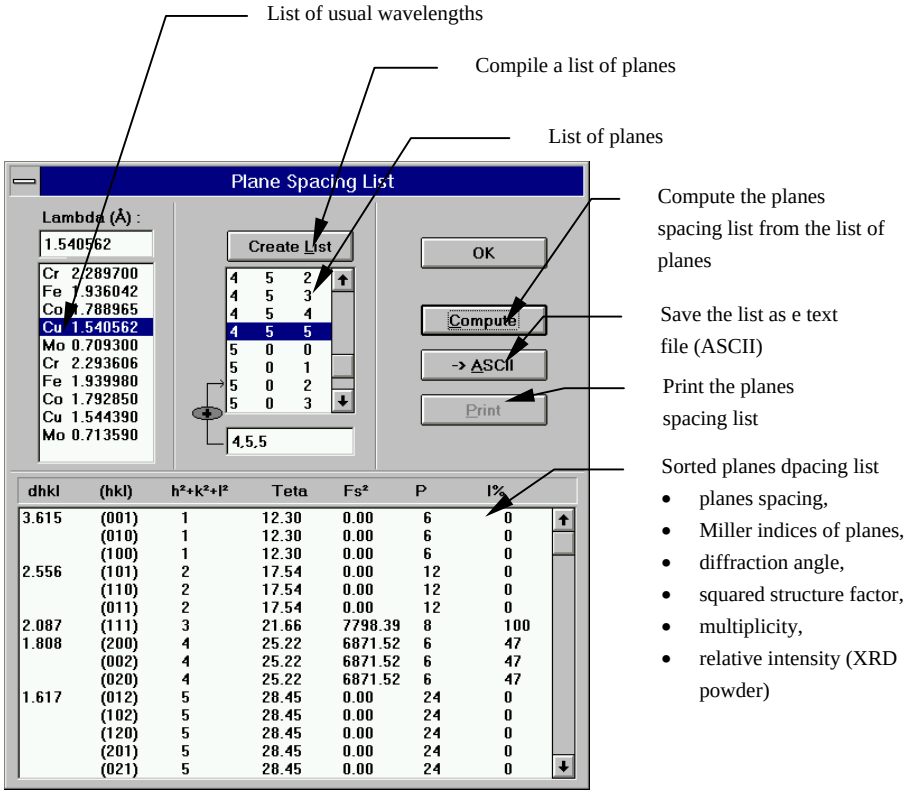
$$d = \frac{4\pi}{3V} \sum_{i=1,N} r_i^3$$

where V is the cell volume and r_i the radius of the i^{th} atom of the unit cell which counts N.

Plane spacing (List)

This function calculates an arranged planes spacing list.

A list of planes should be compiled and then calculated using the button Compute. To obtain the diffraction angle (RX) either the wavelength should be chosen from the available list or its value entered directly into the edit text.



Compute the planes spacing list from the list of planes

Save the list as e text file (ASCII)

Print the planes spacing list

Sorted planes dpacing list

- planes spacing,
- Miller indices of planes,
- diffraction angle,
- squared structure factor,
- multiplicity,
- relative intensity (XRD powder)

F2.12 : Ordered planes spacing list.

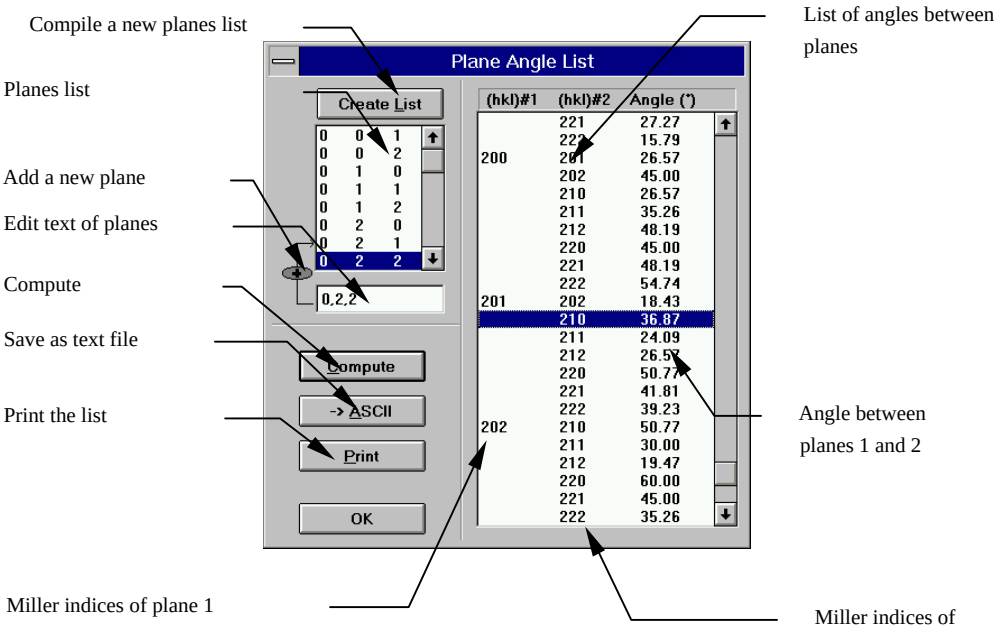
Bragg's angle is calculated by : $\theta = \mathrm{ArcSin}\frac{n\lambda}{2 \cdot \mathbf{d_{hkl}}}$. When $\frac{\lambda}{2 \cdot \mathbf{d_{hkl}}} > 1$, no value is given for θ.

The list compiled in this way can be printed using the [Print] button or saved as a text file (ASCII, [-> ASCII] button).

See Appendix D for a description of the use of the planes list .

Plane angles (List)

This function calculates a list of interplanar angles.
A list of planes should be compiled and then calculated using the [Compute] button. The list compiled in this way can be printed using the [Print] button or saved as a text file (ASCII, [-> ASCII] button).



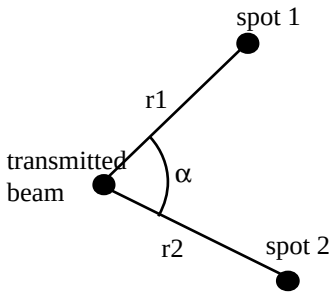
F2.13 : Planes angles list.

See Appendix D for a description of the use of the list of planes.

Identification of planes

CaRIne allows the planes (hkl) to be identified from an approximate knowledge of their inter planar distance and the angle which is formed between them.
The values should be entered in the edit text d_1 and d_2 (in Å) and α (in degrees) and computed using the Compute button. CaRIne gives an arranged list of possible solutions (max. : 100) in ascending order of error. For each solution, the corresponding zone axis is calculated and displayed. From the zone axis, a cut of the reciprocal lattice can be calculated (see Chap.8 "Zone Axis" function). The list can be printed using the Print button or saved as a text file (-> ASCII button).

Application to the indexation of electronic diffraction patterns



F2.14 : Indexation of diffraction patterns.

CaRIne can help with the analysis of electronic diffraction patterns.

Using the measure of the distances r_1 and r_2 between two spots and the beam transmitted, and from the angle α which is formed (see fg F2-14) CaRIne indexes the spots and calculates the corresponding zone axis. CaRIne also provides an arranged list which permits any measurement error of r_1, r_2 and α to be dealt with.

CaRIne proposes various possibilities :

- Either, you yourself have calculated d_1 and d_2 :

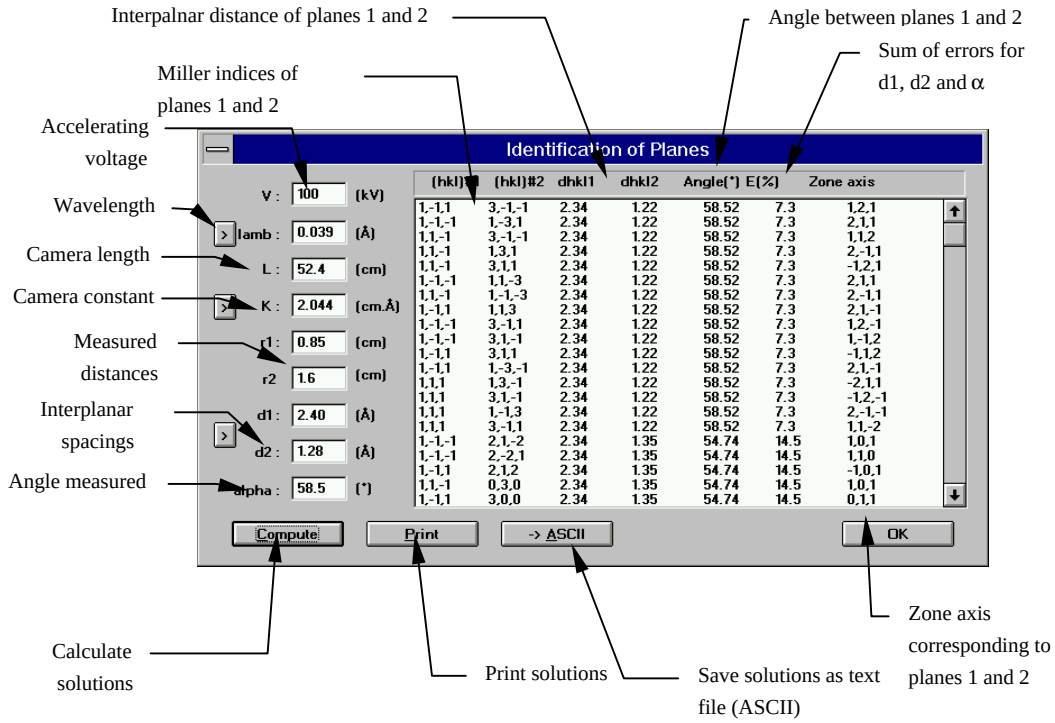
  ⇒ these values can be entered directly into the corresponding edit text (in Å),
  ⇒ next, enter the value of the angle α (in degrees) and click on Compute.

- Or, you know the constant of the camera K and you measure r_1 and r_2. In which case :

  ⇒ enter K (in cm.Å), r_1 and r_2 (in cm) in the appropriate edit text,
  ⇒ click on [>] placed in front of d_1 and d_2, CaRIne then calculates these values (in Å),
  ⇒ enter the angle α (in degrees),
  ⇒ click on [Compute].

- Alternatively, you know the accelerating voltage of the microscope and the camera length. Measure r_1, r_2 and α :

  ⇒ enter the accelerating voltage V in kV,
  ⇒ click on [>] placed in front of λ, CaRIne then calculates the length of the corresponding wave (in Å),
  ⇒ enter the length of the camera L (in cm),
  ⇒ click on [>] placed in front of K, CaRIne then calculates this constant in cm.Å,
  ⇒ enter r_1 and r_2 in cm,
  ⇒ click on [>] placed in front of d_1 and d_2, so that CaRIne calculates these values (in Å),
  ⇒ enter the angle α (in degrees),
  ⇒ click on [Compute].



F2.15 : Indexation of electronic diffraction patterns : list of possible solutions.

The list is arranged with error values in ascending order :

$$\sum(\Delta\%) = 100 \cdot \left(\frac{|d_{1m} - d_{1c}|}{d_{1c}} + \frac{|d_{2m} - d_{2c}|}{d_{2c}} + \frac{|\alpha_m - \alpha_c|}{\alpha_c} \right)$$

where d_{1m} is the measured value of d_1, d_{1c} its calculated value (ditto for d_2 and α).

Formulas used :

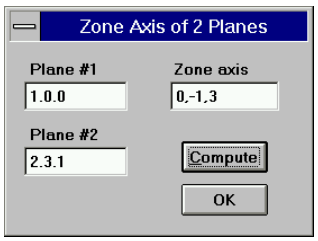
- The wavelength (e^-) : $\lambda = \frac{h}{\sqrt{2 \cdot m \cdot e \cdot V}}$, where h is Planck's constant, m is the mass of electron, e the charge of the electron and V the accelerating voltage.

- The constant of camera K depends on the microscope and possibly the scale of the diffraction pattern. If the diffraction pattern is on a scale of l:l, then K= λ.L where L is the length of the camera and λ the wave length.

- Inter-planar distance : $d = \frac{K}{r}$, where r is the measured value of the diffraction pattern.

Parameters : Search of plane indices up to 10
Maximum individual error accepted on d_1, d_2 and α : 20%

Zone axis of 2 planes

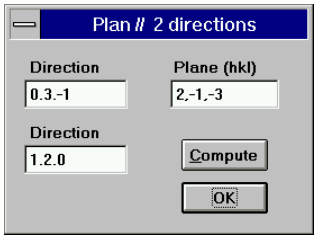


This function calculates the indices u,v and w of the zone axis which corresponds to the data of two planes ($h_1k_1l_1$) et ($h_2k_2l_2$).

The calculation is carried out by pressing the Compute button.

The formula which is used is given in Chap.8 (Reciprocal Lattices).

Plane // to 2 directions



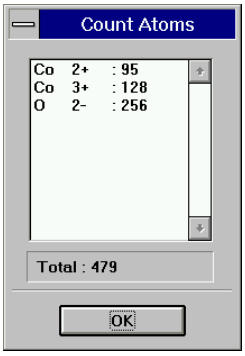
This function calculates the indices h, k, l of the plane which includes the two directions [$u_1v_1w_1$] and [$u_2v_2w_2$].

The calculation is carried out by pressing the Compute button.

The formula which is used is given in Chap.8 (Reciprocal Lattices).

Count Atoms

This function allows the number of visible atoms to be counted by type (same chemical symbol and same oxidation state).



2.8 Menu *Specials*

The Menu ***Special*** regroups the functions which are relative to :

- the study of an atom's environment,
- the visualisation of plane/direction of rolling,
- the X-Ray diffraction patterns,
- the stereographic projection,
- the reciprocal lattices,
- the orientational relationship between several lattices.

Shells

This function shows the successive shells around an atom chosen with the mouse. The atoms which constitute a shell are indicated with a cross. The number of atoms belonging to this shell is given along with the distance from the centre atom. Please note that only atoms of crystal are taken into account. The following shell is obtained by selecting the Next shell button. For each shell, CaRIne gives a "solid angle" (S.A.%) which is calculated by :

$$S.A.\% = 100\ \Sigma(\pi r_i^2) / 4\pi R^2$$

where r_i is the radius of the atoms which constitutes the shell and R the radius of the shell. This number can give an idea of the stability of a structure, for example :

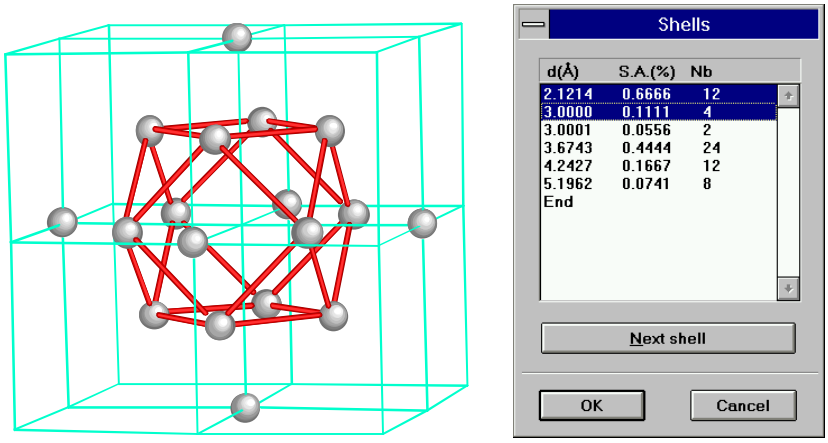
	R(Å)	number of neighbours	S.A.%
Cubic Primitive	1	6	37.5
	1.41	12	37.5
FCC or HCP	1	12	75.0
	1.41	6	18.75

T2.16 : Environment of atoms in a cubic primitive, F.C.C. and H.C.P. structure.

With the help of the mouse, it is possible to select shells by clicking on the calculated list. In this case, only the atoms belonging to these shells will be displayed, the others remaining hidden.

e.g. :

The following drawing shows a FCC lattice (2*2*2 cells). The surrounding of the central atom is being studied. Only the first two shells are selected.

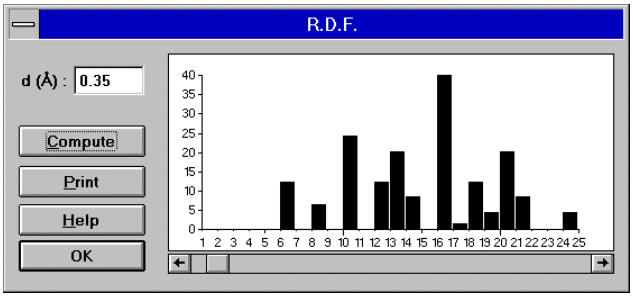


F2.17 : Environment of an atom of the FCC lattice.

The function "**Multi-Link**" Menu ***Lattice*** can be used in order to show the polyhedron edges. Also, the polyhedron function can be used (see 2-31) after having selected one shell, an having made the hidden atoms disappear (function "**Remove all hidden atoms**" / Menu ***Crystal***).

Radial Distribution Function

This command traces the radial distribution function, from a selected atom using the mouse. The result is presented in the form of a histogram. Once a step ("d" in Å) has been chosen, CaRIne distributes the atoms in successive shells and counts the atoms present in each shell. In this way, the first bar of the histogram gives the number of neighbours placed at a distance between 0 and d of the chosen atom. The second bar gives the number of neighbours placed at a distance between d and 2d etc… As for the "**shells**" function, only atoms on the screen are accounted for.



F2.18 : Radial distribution function (FCC 3*3*3 cells)

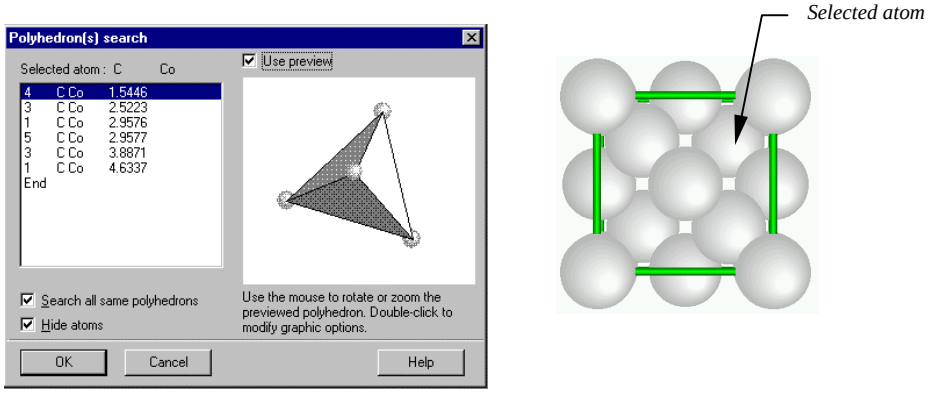
Sphere

This function allows the environment of an atom in a sphere of radius r to be studied. When an atom is chosen with the mouse, CaRIne requests the sphere's radius (in Angstrom), and then hides all atoms which are not contained in this sphere. The radius of the sphere can be determined by the function "**Distance between 2 atoms**" of the Menu ***Calcul***.

Polyhedron

This function searches the coordination polyhedrons of your structures.

The central atom should be chosen with the mouse. CaRIne then identifies the successive layers of neighbours (see F2.19). In the example which is given here (one cell of diamond), there are four first neighbours (covalent carbon) at a 1.54 Å distance , three second neighbours at a 2.52 Å distance etc… With the help of the mouse, select the neighbours which are to be taken into account in order to construct the coordination polyhedron. For this example, only the first four neighbors will be preserved, and will form the summit of the tetrahedron .

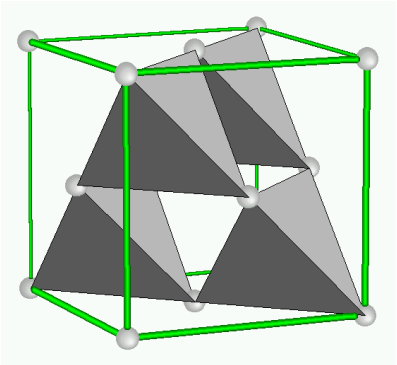


F2.19 : Research of coordination polyhedrons in a diamond cell.

The function *Special/Environment/Polyhedron search* allows to previsualize polyhedron during its construction. Double-click inside the previsualization window to modify the graphic options. Use the mouse (without *Ctrl* key) to rotate the polyhedron or change the scale.

The dialog box "Poly Search" (F2.19) offers two possibilities. The first ("Search all same poly.") enables search, within the whole range of crystal, of the polyhedrons which have the same characteristics as the one you are working on. For example, if the crystal is made up of one diamond cell and this option is chosen, the four tetrahedral sites are obtained at once, as shown in the following figure (F2.20).

The second option ("Hide Atoms") can hide the atoms situated at the summit of the polyhedrons. These atoms can be recalled by using the "**Recall Atom**" function of the ***Crystal*** Menu. The hidden atoms can also be deleted definitively by using the "**Remove all hidden atoms**" function of the ***Crystal*** Menu.



F2.20 : Visualisation of the tetrahedral sites of a diamond cell.

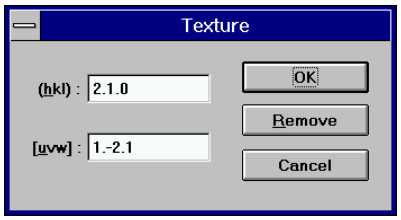
Isolate

This function allows a polyhedron chosen with the mouse to be isolated. Only this isolated polyhedron will be displayed on the screen. In order to visualise the whole crystal the isolated polyhedron should be selected a second time.
For a better visualisation of an isolated polyhedron, it is preferable to place the centre of rotation on the polyhedron's centre atom (see " **Around Atom**" function of the***View*** Menu).

Texture

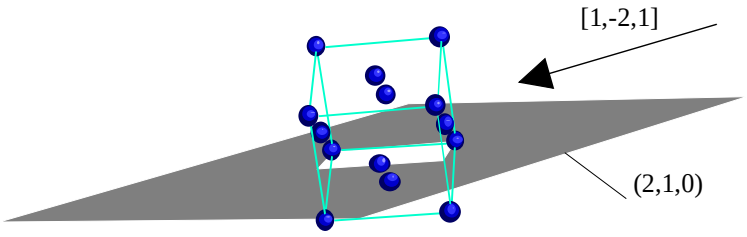
This function provides a graphical representation in perspective of the orientation of a lattice in relation to a direction and a plane (the direction should belong to the plane). The plane corresponds to the plane #1 and the direction is the current direction (see Menu ***(hkl)/[uvw]***).

The intersection of the plane with the structure is calculated on one cell only. The rolling sheet is visualised as a solid rectangle and the intersection as a hole in this sheet.



To cancel this function and return to the original representation, click the Remove button.

e.g. :



F2.21 : FCC in texture view, direction [1 -2 1], plan (2 1 0).

An easy way to define the rolling plane and the direction is to use the function "**? hkl with mouse**" Menu ***hkl/uvw***.
Check the plane #1 is visualised (☒ **hkl planes** check box in Graphics options / Menu ***View***). Then use the function "**? uvw with mouse**" and select two atoms of the plane #1 in order to define the rolling direction. Finally, call the "**Texture**" function and click on OK.

XRD (powder)

This function enables the calculation of the X-Ray diffraction diagram of the current cell (see Chap.7).

Stereographic Projection

This function enables the creation of the stereographic projection of the current lattice (see Chap.6).

Reciprocal Lattice

This function enables the creation of the reciprocal lattice of the current lattice (see Chap.8).

Relation of Epitaxy Ctrl-I

This function allows the orientation relationship between several lattices to be given in order to fix their relative orientation and to superimpose their stereographic projections or their x-ray diffraction diagram. This is done with the study of relationships in matrix/precipitate or substrate/film in mind (see Chap.5).

Associated Lattices Ctrl-L

This function allows real lattices to be associated in order to set their relative orientation and to superimpose their stereographic projections or their diagram of x-ray diffraction. This is done with the study of relationships in matrix/precipitate or substrate/film in mind (see Chap.5).

2.9 Menu *Crystal*

The functions of this menu allow the visualisation of atoms, links and polyhedrons to be acted upon. Any modifications carried out on the structure, using the following functions, only concern the crystal and do not affect the unit cell. For the atoms of the unit cell to be modified the function "**Creation**" must be used (see p 2-13 and Chap.3 : Creation of a new unit cell) or the function "**Crystal to cell**" (see p 2- 13).

Most of the functions which enable punctual modifications of the structure and visualisation of the crystal are accessible by the tool-palette (see Menu ***Windows***). When this is the case, an icon appears in front of the function.

Spread of ... Ctrl-F

This function allows the multiplication of the unit cell for each of the **a**, **b** and **c** directions. To construct a crystal, the following steps should be taken :

⇒ Define the unit cell (Menu ***Cell***) and save it (Menu ***Files***).

⇒ Expand the unit cell (this function) in the three directions.

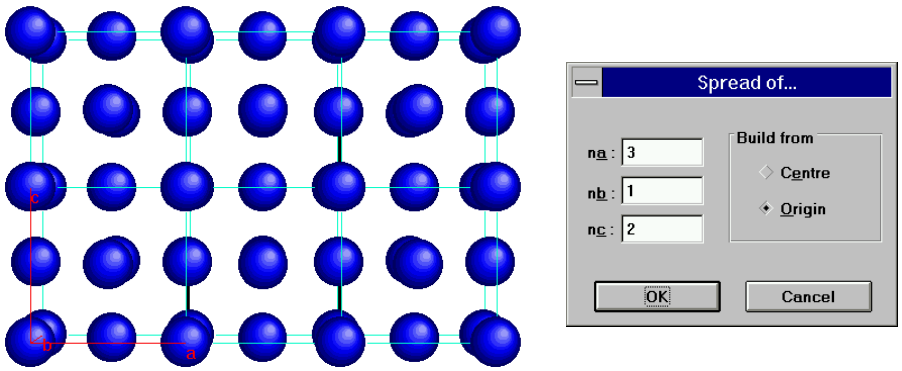
⇒ Modify the crystal (modify links, add or remove atoms, display coordination polyhedrons… Menu ***Crystal***).

⇒ Select the view and save the crystal (Menu ***Files***).

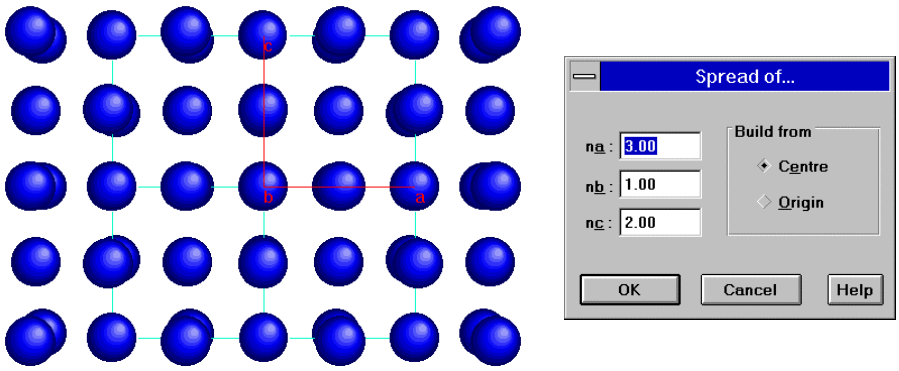
The function "**Spread of ...**" proposes two options. The first one consists in multiplying the unit cell from the original atom situated at a corner of this cell onwards. This multiplication is carried out from a whole number of cells following the directions of the vectors **a**, **b** and **c**. The second option enables the crystal to be spread in 3 dimensions, beginning at its centre. Real values can then be given to the parameters na, nb et nc (see the following example).

Attention : Keep in mind that, due to CaRIne's logic, by modifying the spread of a crystal, previous modifications of the crystal will be lost (unless the function "**Crystal to cell**" has been used, see page 2- 13).

e.g. : Construction in relation to the origin of the unit cell of 3*1*2 FCC cells.



F2.22 : Crystal 3*1*2 FCC cell, built from the origin.



F2.23 : Crystal 3*1*2 FCC cells, built from its centre.

Hide Atom

Click on an atom to hide it. Please note that all hidden atoms can be recalled (they are not erased but saved in "crystal" file). Click a second time on the same position to hide an atom which is behind the first one.

Hide all

This function allows all atoms or all the atoms of a particular type (chemical symbol and degree of oxidation) to be hidden.

Recall

This function recalls a hidden atom. Simply click on the site of a hidden atom to recall it. If another atom is behind the one that has been recalled, click on a second time

Recall all

After confirmation, this function recalls either all hidden atoms or all the atoms of a particular type. Therefore, do not hesitate to use the "**Hide Atom**" function to look in the internal structure of a crystal.

Label

This function enables an atom's label (chemical symbol and level of oxidation) to be displayed or removed, when the atom in question is designated with the mouse (see Chap.4). The labels will only appear if the check box ☒ **Labels** of the "**Graphics**" function is checked.

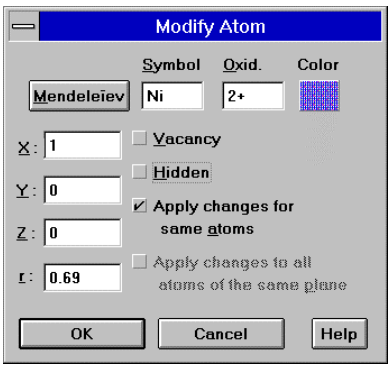
Label all

After confirmation, this function allows all the atom's labels to be displayed. The labels will only appear if the check box ☒ **Labels** of the " **Graphics**" function is checked.

Modify Ctrl-M

By clicking on an atom, it is possible to obtain all its attributes :

- chemical symbol and level of oxidation,
- the co-ordinates x,y,z in the frame (**a**,**b**,**c**),
- the radius (in Angstrom),
- the colour,
- hidden or not,
- vacancy or full site.



F2.24 : Modifying an atom.

It is then possible to change all this information. This function can be used to displace an atom (to illustrate relaxations or dislocations, for example) or for example to perform a substitution (using Mendeleev's table). This is the basic function to be used to represent point defects. To modify the colour, click on the *colour box* . All atoms identical to the one selected (same chemical symbol, level of oxidation, colour and radius) can be modified by crossing off the ☒ **Apply for all same atoms** check box.

If the atom belongs to the plane n°1 (see ***hkl/uvw*** Menu), and you wish to modify all the atoms of this plane, cross off the ☒ **Apply for plane #1** check box. The stacking of planes can rapidly be displayed by giving a particular colour to the atoms of any same plane (see example 2, Chap.9).

Add Ctrl-A

This function enables an atom to be added, particularly in an interstitial position. The following steps should be taken :

⇒ it is advisable to display the frame (**a**,**b**,**c**) or (**x**,**y**,**z**) (this helps to find one's bearing within the lattice),

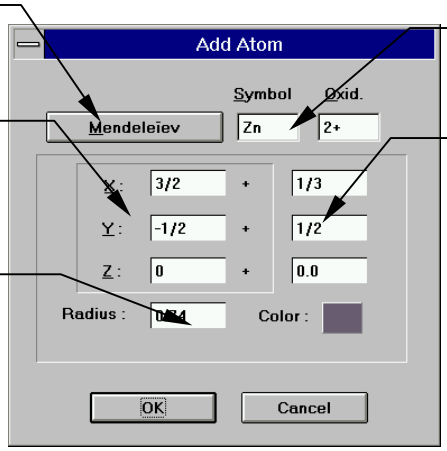
⇒ as adding an atom is relative to a full site, select an atom close to the interstitial site, with the mouse,

⇒ enter the coordinates of the vector included between the selected atom and the new atom you would like to add.

Access to Mendeleev's table

Coordinates of selected atom within the frame (**a**,**b**,**c**)

Atomic radii of new atom



Chemical symbol, level of oxidation and colour of new atom

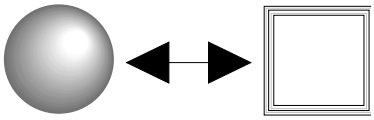
Coordinates of the translation vector within the frame (**a**,**b**,**c**)

F2.25 : Adding an atom.

Please Note: With this function, it is possible to create all types of structure, including organic molecules.

Vacancy

This function replaces an atom, designated with the mouse, with a vacancy (or a vacancy with an atom). A vacancy is represented by a bicolour square (i.e. black and the colour of the atom).



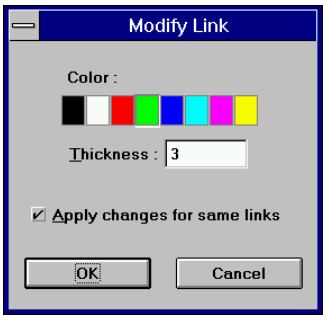
Remove

This function allows an atom (and its links) chosen with the mouse, to be removed. Contrary to the " **Hide**" function, this is irreversible and the atom is erased from memory.

Remove Hidden

After confirmation, this function allows all hidden atoms (and their links) to be removed. These atoms are then no longer accounted for by CaRIne. This accelerates computing and reduces the size of the corresponding crystal file.

Modify link



F2.26 : Modification of a link.

This function enables a link between two atoms to be modified using the mouse. If you wish to apply these modifications to all connections of the same colour and thickness as those designated cross off : ☒ **Apply changes for same links**.

Remove

This function allows the link existing between two atoms, designated with the mouse, to be removed (irreversible).

Remove all

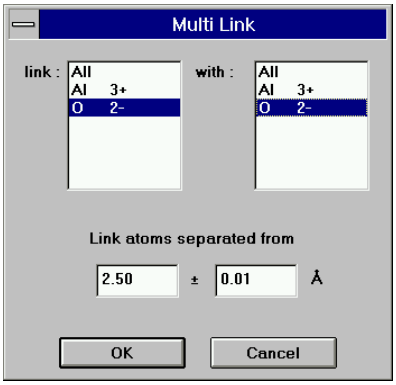
After confirmation, this function allows all links of a crystal to be removed (irreversible).

Add

This function allows two atoms, designed with the mouse, to be linked. The colour and thickness of a new link are defined in the "**Preferences**" function.

Multi link

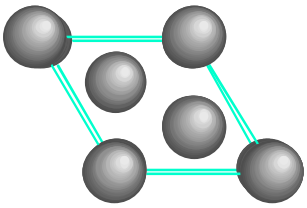
This function enables certain atoms separated by a distance d (± epsilon) to be linked. The choice of atoms to be linked is made according to their chemical symbol and their oxida-tion state.



F2.27 : "Multi Link" Function.

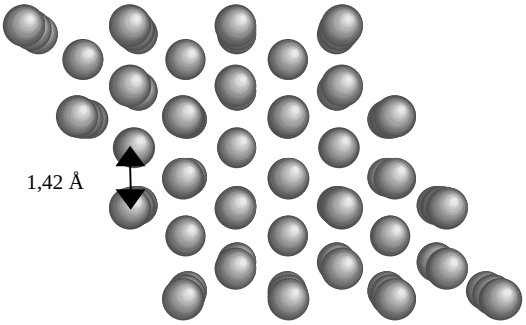
Example : Visualisation of the lamellar structure of graphite.

⇒ After loading of the graphite motif, an unit cell is obtained.

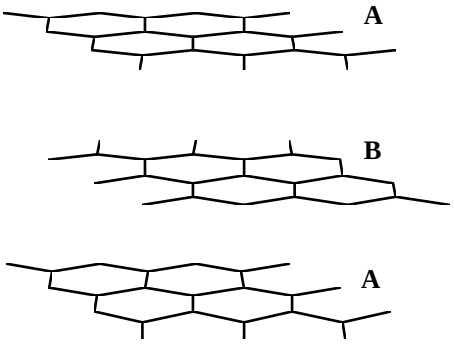


⇒ In order to show the stacking AB of graphite, the lattice should be spread to 3*3*1 cells, and then all links should be removed.

⇒ Ask for the distance between two atoms which form the edge of one of the hexagons (you should obtain 1.42 Å).



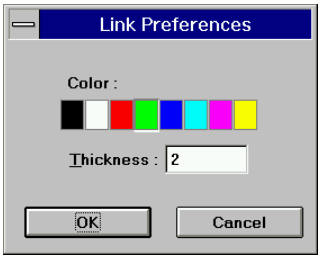
⇒ Choose " **Multi Link** ", the measured distance will appear as the default distance click on OK button. After rotation around xx', the stacking of the planes ABAB can be visualised.



Preferences

This function allows the colour and thickness of each new link to be chosen. Before creating a new structure (***Cells*** Menu), it is through this function that the type of link which will form a frame can be chosen. By default, the colour will be black and the thickness will be one.

For the thickness of links, it is preferable to use values comprised between 0 and 10. The value 0 allows a minimum thickness, independent of the scale, to be obtained.



F2.28 : Links prefs.

Modify Polyhedron

This function allows a polyhedron, designated with the mouse, to be modified. All polyhedrons identical to the one chosen (same colour and number of sides) can be modified by using the ☒ **Apply to all similar polyhedrons** check box.

Possible modifications : colour of the sides, colour of the edges, hidden or not.

Hide

Click on a polyhedron in order to hide it. Note that all hidden polyhedrons can be recalled (they are not erased from memory but saved in a "crystal" file. Click a second time on the same place to hide a polyhedron behind the first.

Recall

This function enables a hidden polyhedron to be recalled. Simply click on the site of a hidden polyhedron to recall it. If another hidden polyhedron is to be found behind this one, click on a second time.

Recall all

After confirmation, this function recalls all hidden polyhedrons.

Remove

This function allows a polyhedron, designated with the mouse, to be removed from memory.

Remove hidden

After confirmation, this function removes all hidden polyhedrons from memory.

Label

This function allows the label of a polyhedron, designated with the mouse, to be displayed or removed (chemical symbols and oxidation state for atoms of summits and for the polyhedron's centre atom).

Label all

After confirmation, this function allows all the polyhedrons' labels to be displayed.

2.10 Menu *View*

The functions of this menu allows the scales of the real or reciprocal lattices and the parameters of the crystal rotation to be modified.

Graphics Ctrl-G

This function enables modification of the graphical representation of the current crystal, the stereographic projection, the x-rays diffraction diagram or the reciprocal lattice (see §4.5).

Note : The " **Graphics**" function opens the appropriate dialogue box according to the type of window in use.

General Scale Ctrl-E

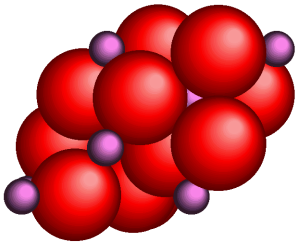
Modifies the size of all objects displayed on the screen by entering a value for the general scale. This value is proportional to the size of the objects. The general scale should is between 1 and 2000. This function is applied to all real and reciprocal lattices.

Radii Scale Ctrl-X

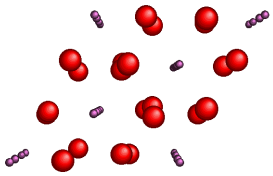
This function is applied to all real and reciprocal lattices. The atoms size of a crystal or reciprocal lattice nodes can be modified independently of the other objects.

This allows compact views (radii scale = 100%) or spread views (radii scale < 100%) to be obtained. The value of this scale parameter must be between 1 and 400%.

Example :



Compact view of Al_2O_3
Radii Scale=100%



Spread view of Al_2O_3
Radii Scale=25%

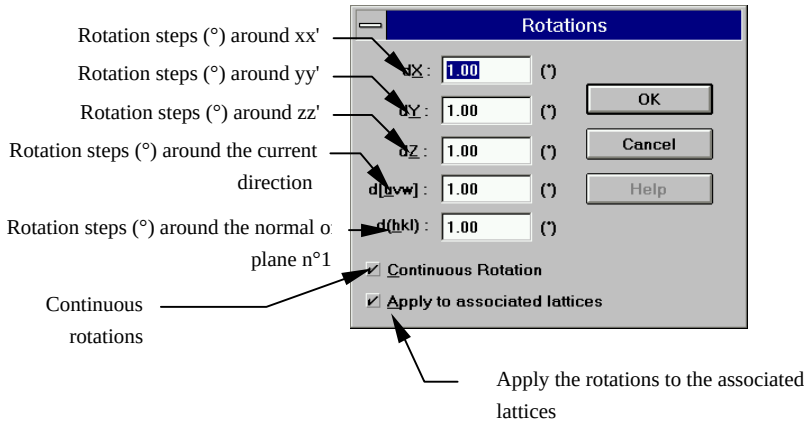
F2.29 : Radii scale.

Zoom ±

These two functions give the same result as the function " **General Scale** ". They are, however, easier to use when adapting the size of a crystal to the size of a window, especially by using the short keys (keys **+** and **-**). "**Zoom +**" corresponds to a multiplication of the general scale by 1.15 and " **Zoom -**" by 0.85. Note that it is possible to pass through a crystal (try a few "**Zoom+**"!).

Keyboard Rotations Parameters Ctrl-R

This function enables rotation steps around 5 axes to be set (see Chapter 4.2 : Lattice rotations); the continuous rotations function to be activated (☒ **Continuous Rotations**); and the same rotations to be applied to the associated lattices (☒ **Apply the rotations to the associated lattices**) (see Chapter 5 : Associated Lattices). The value of rotation steps should be given in degrees.



F2.30 : Rotations parameters.

The rotations are applied using the keys of the numerical keyboard (see Chapter 4).

Around 1 Atom

This function allows the centre of rotation to be moved to the centre of an atom, designated with the mouse.
This function is particularly useful when a polyhedron has been isolated ("**Isolate**" function of ***Special*** Menu) and one wishes to rotate it around its centre, in order to observe its shape.

Around Centre

This function allows the centre of a crystal to be defined as the centre of rotation. It is usually used after the preceding function.

2.11 Menu *Windows*

This menu allows the organisation of CaRIne's windows.

Refresh

Refreshes the active window. This function should be used, for example, after hiding or recalling atoms, or adding links and polyhedrons.

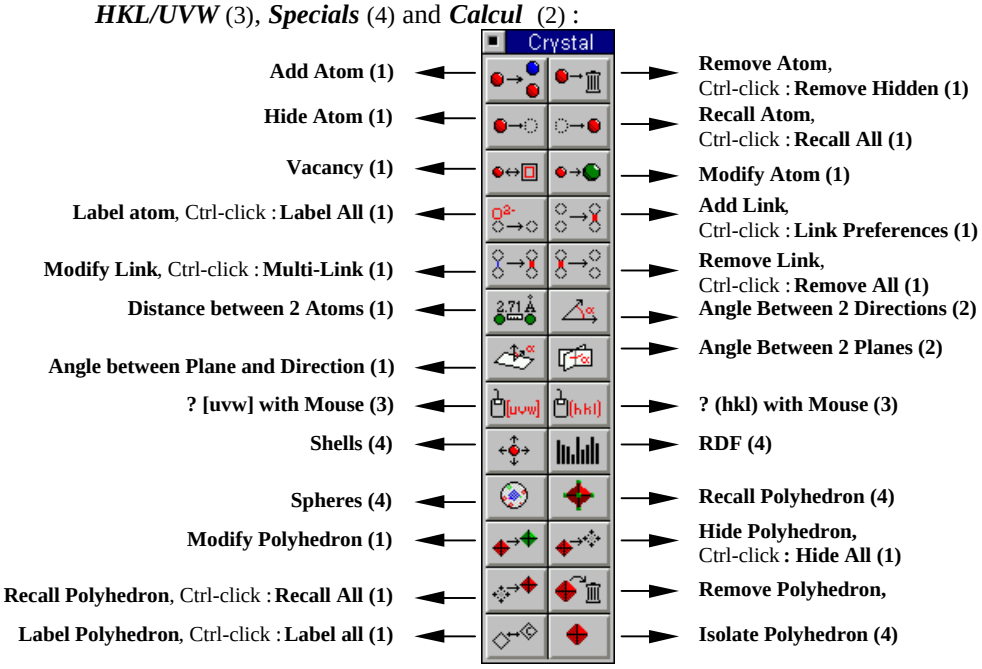
General Tools

This function allows the General Tools palette to be displayed or hidden. This toolbox allows a qwick access to the functions listed below (ordered from left to right) :

Files | New
Edit | Copy picture
Edit | Undo/Redo
Files | Print
Files | Print Preview
Cell | Creation/List
Cell | Space groups
Crystal | Spread of...
Special | XRD | Creation
Special | XRD | Preferences
Special | XRD | Save XRD as ASCII file
Special | Stereo. proj. | Creation
Special | Stereo. proj. | Parameters
Special | Reciprocal lattice | Creation
Special | Reciprocal lattice | Spread of...
Special | Reciprocal lattice | Zone axis

Crystal Tools

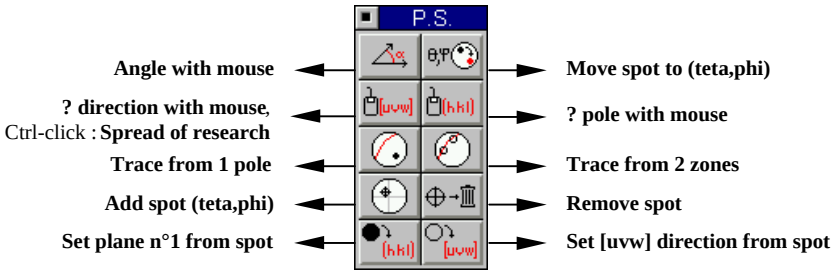
This function allows the Crystal Tools palette to be displayed or hidden. This palette allows rapid access to the functions of Menus ***Crystal*** (1), ***HKL/UVW*** (3), ***Specials*** (4) and ***Calcul*** (2) :


Crystal
Add Atom (1)
Hide Atom (1)
Vacancy (1)
Label atom, Ctrl-click : Label All (1)
Modify Link, Ctrl-click : Multi-Link (1)
Distance between 2 Atoms (1)
Angle between Plane and Direction (1)
? [uvw] with Mouse (3)
Shells (4)
Spheres (4)
Modify Polyhedron (1)
Recall Polyhedron, Ctrl-click : Recall All (1)
Label Polyhedron, Ctrl-click : Label all (1)
Remove Atom, Ctrl-click : Remove Hidden (1)
Recall Atom, Ctrl-click : Recall All (1)
Modify Atom (1)
Add Link, Ctrl-click : Link Preferences (1)
Remove Link, Ctrl-click : Remove All (1)
Angle Between 2 Directions (2)
Angle Between 2 Planes (2)
? (hkl) with Mouse (3)
RDF (4)
Recall Polyhedron (4)
Hide Polyhedron, Ctrl-click : Hide All (1)
Remove Polyhedron,
Isolate Polyhedron (4)

F2.31 : Crystal tools palette

Stereo.Proj. Tools

This function allows the stereographic projection tool palette to be displayed or hidden. This palette allows rapid access to the functions of the Menu ***Special/Stereo.Proj.*** :



F2.32 : Stereographic Projection tools palette.

Rotations Tools

Allows the rotations tools palette to be displayed or hidden (see Chap. 4).

Cascade

This function allows the various windows to be arranged in the form of a cascade.

Tile

This function allows the various windows to be arranged in the form of tiles.

...

A window can be activated with the function of the same name.

CHAPTER 3
Selection of a crystalline structure

3

CaRIne offers four ways of creating crystalline structures. The first way is to use the crystal or cell libraries. It is also possible to use the pre-defined Bravais lattices, or to create your own motifs or unit cells.

3.1 Loading a motif, a unit cell or a crystal from the libraries

CaRIne is delivered with numerous unit cell and crystal files (see Appendix B). They can be loaded simply by using the corresponding commands (see ***Files*** Menu). These files can be modified. The libraries can be enlarged with your own creations. All your work can be saved, from the creation of a unit cell (a, b, c, α, β, γ, atoms and their positions), to the construction made from the cell (what we call a crystal). It is therefore possible to save as many crystals from the same unit cell as you wish. The different steps of a complicated construction can also be saved. With this method, in case of any problem, it is easy to recall the previous version in order to continue your work.

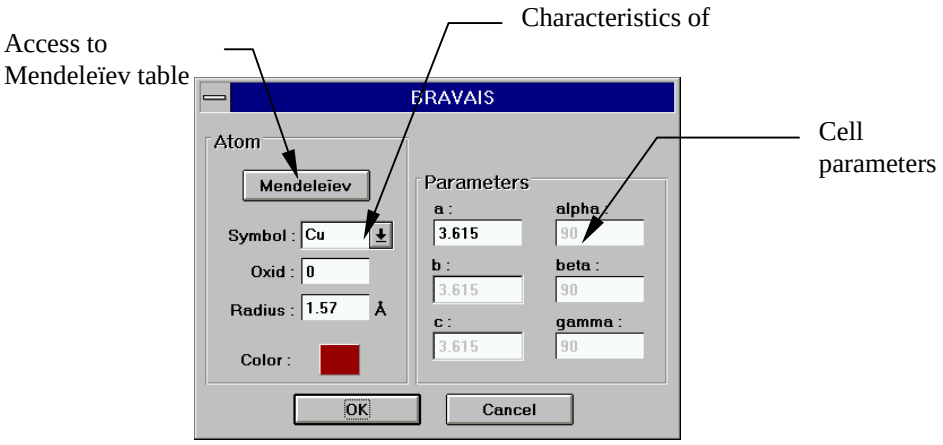
It is possible to import motifs, cells or crystals in the form of ASCII files (see ***Files*** Menu). These structures can then be visualised, modified, printed or inserted into documents. The formats of cells and crystals files are given in Appendix A. This method can be used to visualise structures

whose atomic positions have been previously computed, for example, by a molecular dynamics program.

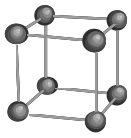
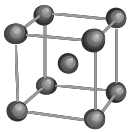
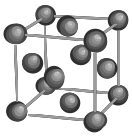
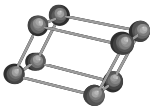
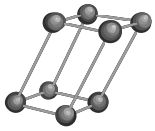
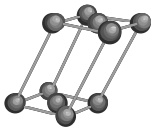
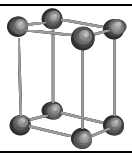
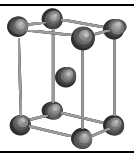
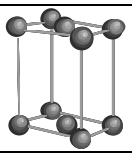
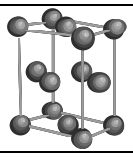
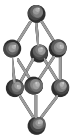
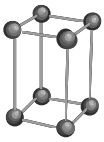
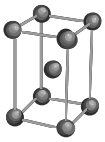
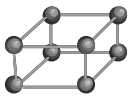
This function also enables cell and lattice files from versions 2.x for MS-DOS and 3.0 for Macintosh of CaRIne, to be imported.

3.2 Use of Bravais' Lattices

It is possible to obtain an example of each of the 14 Bravais lattices within just a few seconds. These functions are grouped together in the ***Cells*** Menu. This is a quick and easy way of illustrating crystalline systems. It is also a quick way of setting the α, β and γ angles of a new cell. The cell can then be accessed and modified by the function "**Creation**" of the ***Cells*** Menu (see following paragraph).
CaRIne automatically sets the cell parameters according to the system which is chosen. Here, since the crystalline system is cubic, a value can only be given for a (b and c being equal to a, and, α β and γ set at 90°).



Use of Bravais' Lattices

	Primitive (P)	Body-centred (I)	Base-centred (C)	Face-centred (F)
Cubic a=b=c α=β=γ=90°				
Triclinic a≠b≠c α≠β≠γ				
Monoclinic a≠b≠c α=β=90° γ qcq				
Orthorhombic a≠b≠c α=β=γ=90°				
Trigonal a=b=c α=β=γ≠90°				
Tetragonal a=b≠c α=β=γ=90°				
Hexagonal a=b≠c α=β=90°γ=120°				

When these functions are used, CaRIne places an atom at each node. If one doesn't want an atom at (0,0,0), the "Space Groups" function should be used (see §3.4).

Note : Please note that once a Bravais lattice has been called, CaRIne loses all memory of the lattice which has been selected. If an atom is then added by the function "**Creation**" (see §3.3), it will not be duplicated on the equivalent sites of the lattice. If one wishes to obtain this effect, the space groups must also be used (see §3.4). For example, to create NaCl from an atom of Na^+ at (1/2,0,0) and an atom of Cl^- at (0,0,0), the group $Fm\bar{3}m$ should be used and not the cubic face-centred function.

3.3 Construction of a new unit cell

It is possible to access cell parameters as well as the list of atoms of the motif at any time, by using the function "**Creation**" of the ***Cells*** Menu. A quick way of pre-defining cell parameters according to the system is to use the Bravais lattices functions before calling the function "**Creation**".

To create a new unit cell, the position of each atom must be known. Mendeleev's table can be used to give their characteristics separately (chemical symbol, level of oxidation, radius, colour and occupancy). The cell can comprise several thousand atoms.

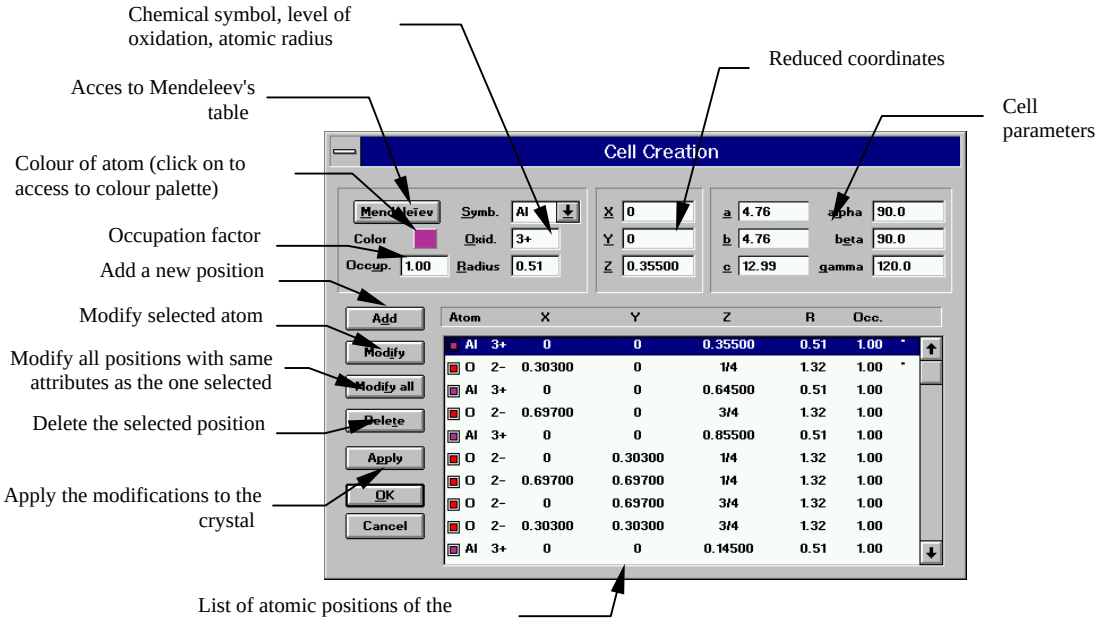
The dialogue box of the unit cell is comprised of 6 edit texts for the cell parameters (a, b, c, α, β, γ), a list of atomic positions, 7 edit texts for entering positions (chemical symbol, level of oxidation, x, y, z, r, occupation factor). One button allows an atom's colour to be modified and 4 buttons enable an atomic position to be added, modified or removed.

The occupation factors enables a percentage of vacancies to be given, this should be between 0 and 1 and is used to calculate X-ray diffraction diagrams.

The atomic positions are reduced coordinates (between 0 and 1) and can be entered in the form of fractions. The use of fractions is useful in order to benefit from CaRIne's precision : **1/100 000**.

To edit an atom's characteristics, the line to be modified should be chosen with the mouse, then the changes made in the edit texts situated at the top of the window, and next click on [Modify] or [Modify all] buttons.

Note : *the parameters a, b, and c should be given in Angstrom; α, β and γ in degrees.*



Note : When a crystalline system is selected (see previous paragraph), default values are given for a,b,c, α,β,γ. These values can be modified, CaRIne will automatically search for the corresponding crystalline system and display it in the status bar (see Chap.2 §2.1).

Description of the different buttons :

- Add : Add a new position to the unit cell.

- Modify : Modify the selected position (Attention : It is not sufficient to modify the values in the edit texts, this must be confirmed by using Add or Modify buttons).

- Modify all : Modify all the positions with the same attributes as the one which has been selected. i.e. modify a position if it has the same chemical symbol, level of oxidation, radius and colour as the position selected.

- Delete : Delete the selected position.

- Apply : Apply the modifications to the crystal without quitting the dialogue box. The modifications are also applied to the reciprocal lattice, the stereographic projection and to the x-ray diffraction diagram; if these exist. This function will allow you to see the consequences of the modifications you are applying, step by step.

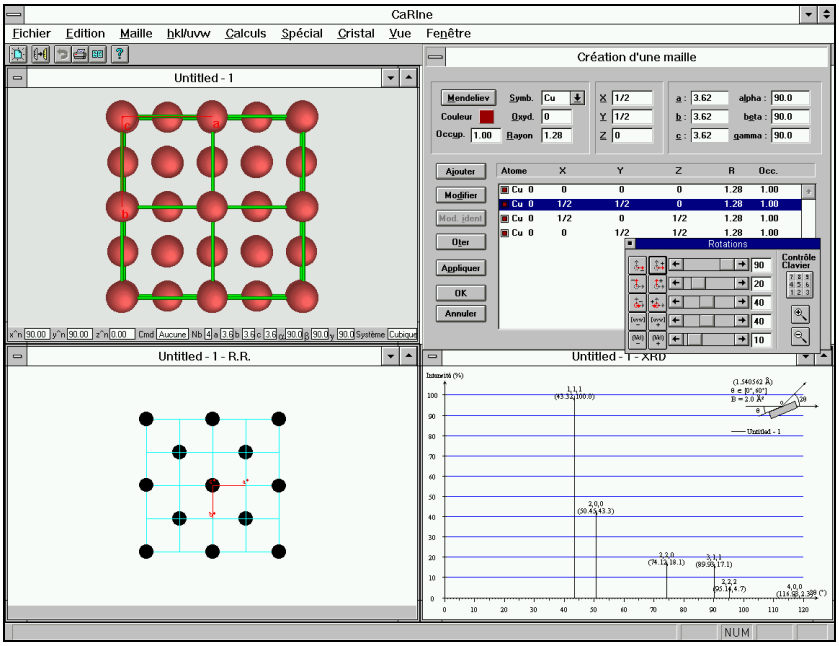
- Cancel : Cancel all modifications made to the unit cell since the "Creation" dialogue box was opened.

The *Creation/list* dialog box can be moved or resized with the mouse. All these parameters are saved in the registry.

Header-controls have been added inside this dialog box for the display of the atom/position list.

The Rotations tool palette can be used when the *Creation/List* dialog box opened (see Chap 4.2.5). This is useful when building a new cell and using the *Apply* button. If rotation tools are not visible, you can recall it by pressing the *Ctrl* key of the keyboard and clicking on the *Apply* button.

In order to immediately visualise the modifications due to changes to the unit cell, it is advisable to set out the windows as follows :



With this method, the modifications will be visible in all the windows associated with the real lattice.

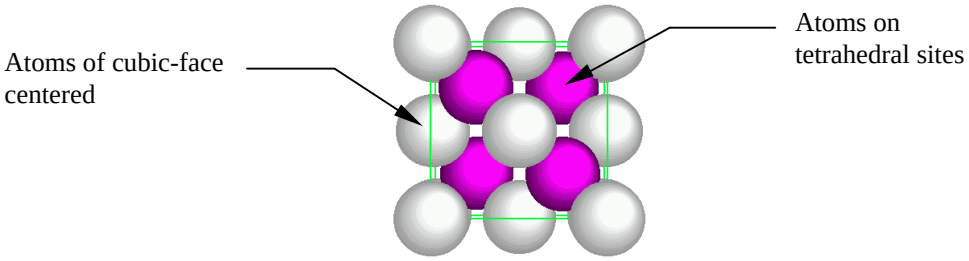
Example of cell definition : The diamond unit cell.

The diamond cell consists of a FCC cell with an atom of carbon at (0,0,0) and with four additional atoms on the tetrahedral sites. The coordinates of these atoms are :

X	Y	Z
1/4	1/4	1/4
3/4	3/4	1/4
3/4	1/4	3/4
1/4	3/4	3/4

To create the diamond unit cell, simply follow this sequence :

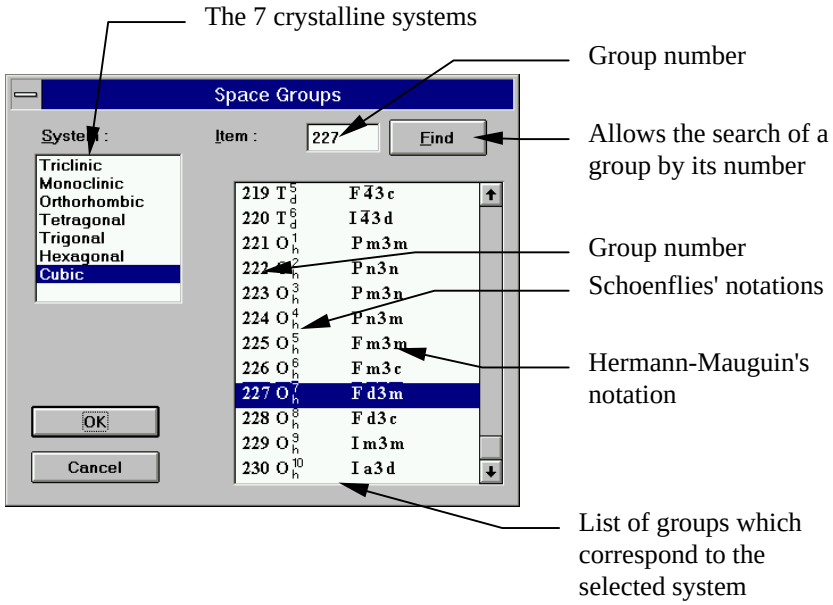
⇒ "**New**" from the ***Files*** Menu, a new window appears,
⇒ "**Cubic - Face-Centred**" from the***Cells*** Menu, enter 3.567 Å for **a**, choose the carbon atom from the Mendeleev's table,
⇒ "**Creation**" from the ***Cells*** Menu, add the four atoms on tetrahedral sites, when this is done, you should obtain the following :



Remark : using the " **Space groups** " function one can also define the diamond lattice from the space group 227 ($Fd\bar{3}m$) with only one atom at 1/8,1/8,1/8.

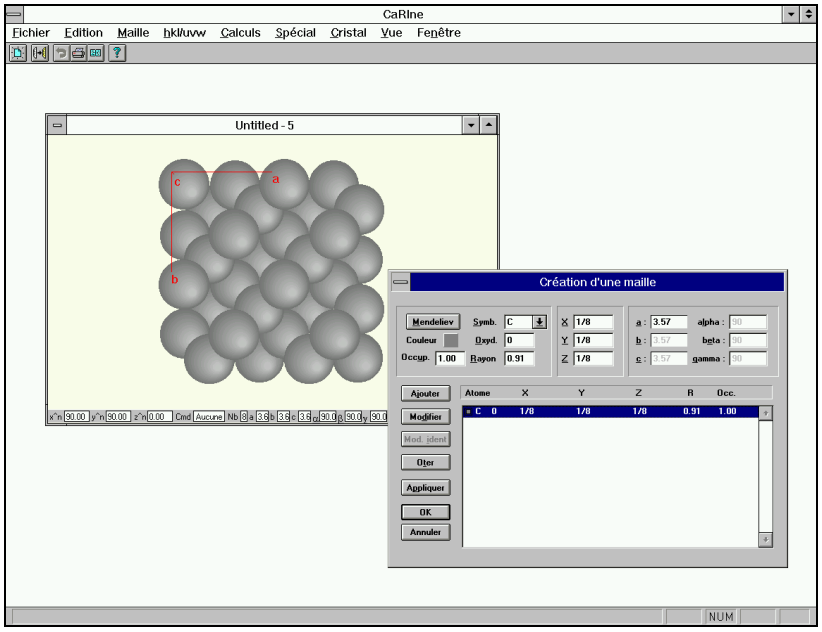
3.4 Space Groups, construction of a new motif

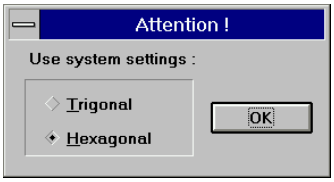
The " **Space Groups** " function of the ***Cells*** Menu enables the construction of a unit cell from a motif and a space group.



The space groups are classified according to the seven crystalline systems, in order of the group number in Schoenflies 'notation. For each group Hermann-Mauguin's notation is also given.

Once the space group has been selected, a dialogue box is opened in order to enter non-equivalent positions (i.e. the motif). This box also enables cell parameters (a, b, c, α, β, γ) to be attributed to the structure. As with Bravais lattices the cell parameters are set according to the system which is chosen.





For the space groups 146, 148, 155, 160, 161, 166 , 167 and for all the space groups of trigonal system , the choice of whether to use hexagonal or rhomboedral descriptions is left to the user.

The use of the dialogue box which allows the motif to be entered is described in the previous paragraph.

The choice of space group, the cell parameters and the motif define the unit cell. It is then possible to visualise the resulting positions of all the cell's atoms by using the function "**Creation**" of the ***Cell*** Menu (the non-equivalent positions are marked with an asterix, see § 3.3).

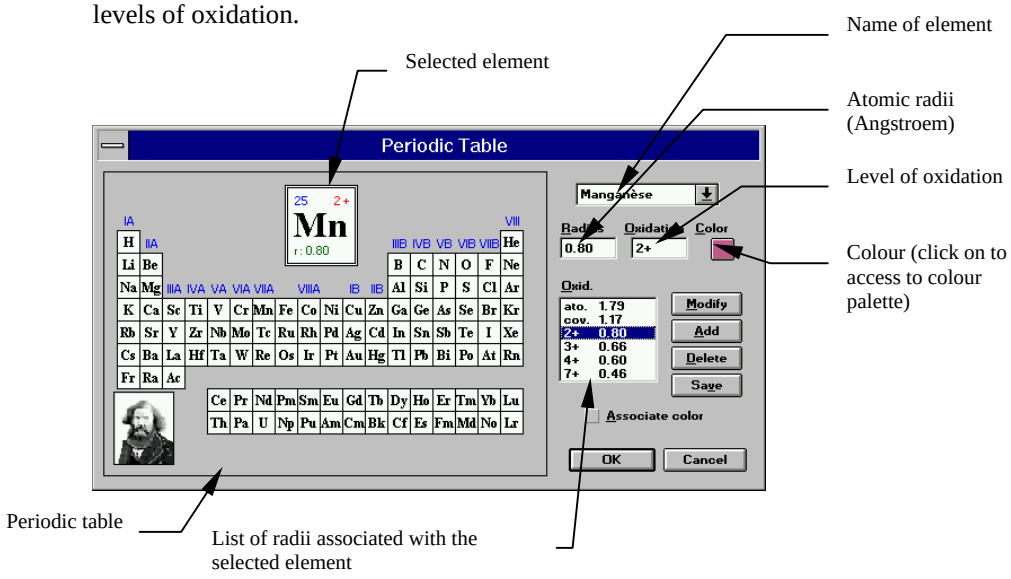
CaRIne conserves in memory the number of the space group and the list of non-equivalent positions. In this way, if a group and a motif have previously been defined, it is possible to re-edit them by recalling the "**Space Groups**" function (attention : this is only possible if the unit cell

positions have not been modified in the meantime by the " **Creation**" function or "**Lattice to Cell** " function). The space group and the list of non-equivalent positions are also saved in the cell files (***Files*** Menu).

The figure F1.2 (Chap.1) summarises the way in which the concepts motif, cell, lattice are connected within the program.

3.5 Use of Mendeleev's table (Periodic table of elements)

CaRIne offers the use of Mendeleev's table when a new lattice is created; when an atom is modified or added. Each of the elements of the table is given with a colour and a list of atomic radii corresponding to their levels of oxidation.



Name of element

Selected element

Atomic radii (Angstroem)

Level of oxidation

Colour (click on to access to colour palette)

Periodic table

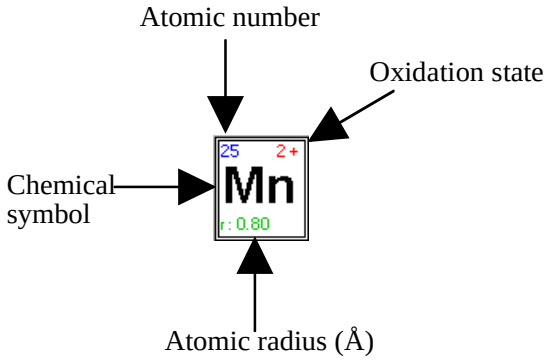
List of radii associated with the selected element

Each element of the table can be modified separately, either by modifying the pre-defined colour or by adding or removing radii from the list. To save these modifications, click on the Save button.

An element is chosen by clicking on the corresponding box; the radius and level of oxidation are chosen by clicking on the **list** of radii or by entering directly the values into the edit texts **Radius** and **Oxidation.**

Note : *The valence of a covalent atom is specified by the symbol Co instead of the level of oxidation state.*

The selected element is displayed at the top of the table with the following characteristics : chemical symbol, atomic number, radius and oxidation state.



Note : *If at least one element of the table has been modified, CaRIne allows the modifications made to be saved.*
An error message appears if the Mendeleev's table is not in the same folder as CaRIne (see Installation Procedure Chap.0).

CHAPTER 4
Visualisation functions

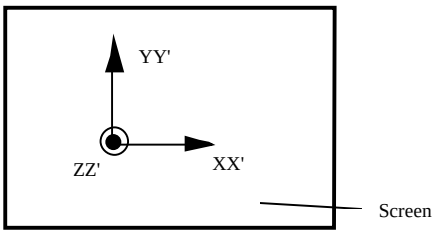
4

The visualisation functions are composed of rotations, projections, scales and the selection of different objects to be displayed.

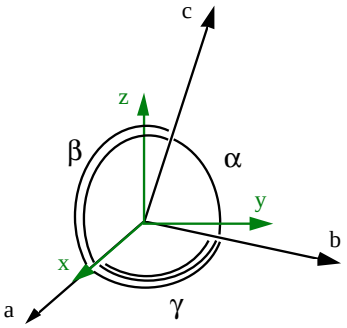
4.1 The different reference frames of CaRIne

CaRIne works with three different reference frames in 3-D :

- A reference frame linked to the screen, R_e
- An orthonormal reference frame which rotates in Re, R_r or (**x**,**y**,**z**)
- A reference frame linked to the unit cell, R_m or (**a**,**b**,**c**).



The reference frame linked to the screen (R_e) is fixed. It is used as a reference for rotations from the keyboard. The ZZ' axis is perpendicular to the screen, the YY' axis is vertical and the XX' axis is horizontal.



The reference frame (R_m) is defined as fixed within the reference frame (R_r) by the cell parameters (a, b, c, α, β, γ). (Rm) is formed of the triplet cell vectors (**a**,**b**,**c**).

4.2 Rotations

CaRIne allows a real lattice, a reciprocal lattice or a stereographic projection to be orientated in five different ways.

Note : The centre of rotation is defined by the functions " **Around 1 Atom**" and " **Around Centre** " of the ***View*** Menu. The first of these functions enables the rotation of a crystal around an atom which has been selected with the mouse. The second redefines the centre of the crystal as being the centre of rotation.

4.2.1 Using Miller indices

The first is based on the Miller indices. A lattice can be projected either following a direction or perpendicularly to a plane. These projections lead to the direction [uvw] or the normal to (hkl) plane on the ZZ' axis of the screen reference frame (R_e) (see ***hkl/uvw*** Menu).

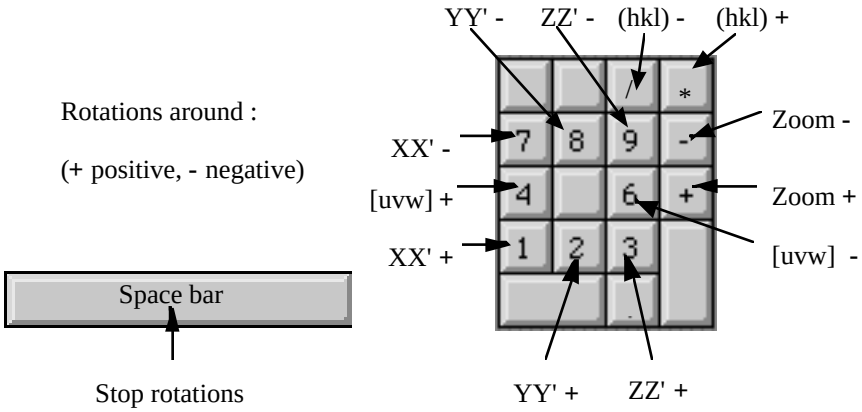
4.2.2 Using the keyboard

The second way is to orientate, from the keyboard, the reference frame (R_r), and thus the lattice, the stereographic projection and the reciprocal lattice. These rotations are carried out within the screen reference frame (R_e) around five axes : three of which are the XX', YY', ZZ' of (R_e); the fourth, the axis defined by the direction [uvw] (see ***hkl/uvw*** Menu) which

passes through the centre of the lattice; and the fifth, the axis defined by the normal to plane #1, which passes through the centre of the lattice. The [uvw] direction and the (hkl) plane #1 can be defined using the mouse (see ***hkl/uvw*** Menu).

The keys to use are :

- <**1**> and <**7**> to rotate around the XX' axis,
- <**2**> and <**8**> to rotate around the YY' axis,
- <**3**> and <**9**> to rotate around the ZZ' axis,
- <**4**> and <**6**> to rotate around the axis defined by the [uvw] direction,
- </> and <*****> to rotate around the axis defined by the normal to plane n°1.



If continuous rotation is required, the box ☒ **Continuous Rotations** ("**Rotations**" function / Menu ***View***) should be crossed off. In this case each time one of these keys is pressed, the speed of the rotation is increased or decreased by the value of the rotation step of the corresponding axis. To stop the rotations, press the **<Space Bar>** key. The angles between the **x,y,z** axes of R_r and the normal to the screen are indicated in the status bar (see Chap.2 - §2.1). These values are given after the symbols : x^n=..., y^n=..., z^n=....

4.2.3 Using the mouse

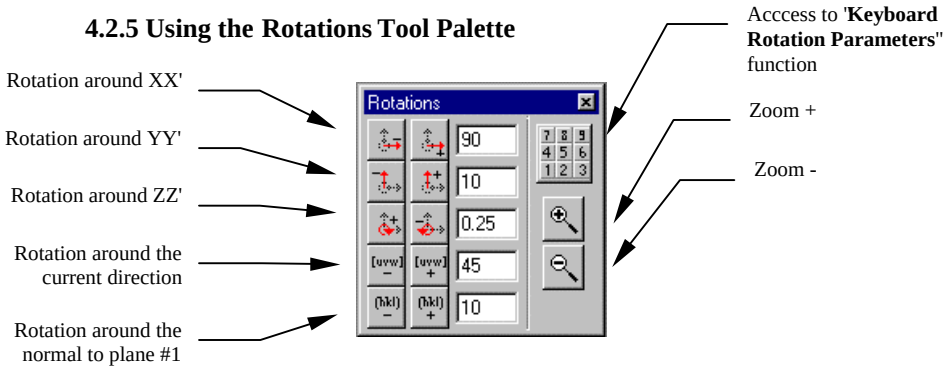
It is also possible to rotate the crystal or modify the scales using the mouse. Try to move the mouse and press simultaneously the *Ctrl* key of your key-board and the left button, then with the right button and finally with both buttons. Those combinations permit to turn around the 3 axis and allow to zoom.

keyboard	mouse button	mouse movement	effect
Ctrl	right	move around	rotations around zz’
	left	move around	rotations around xx’ and yy’
	right and left	up and down	zoom (general scale)
Ctrl + Shift	right	move around	*no effect*
	left	move around	*no effect*
	right and left	up and down	zoom on radii (radii scale)

4.2.4 Using the stereographic projection

Real and reciprocal lattices can be orientated with the help of the stereographic projection (see Chap.6).

4.2.5 Using the Rotations Tool Palette



The rotations tool palette enables access to the functions of the ***View*** Menu. It also enables the same rotations to be carried out as with the keyboard, by using the corresponding icons, as well as the modification of the scales of real and reciprocal lattice.

The Rotations tool palette can be used when the *Creation/List* dialog box is opened (see Chap 3). This is useful when building a new cell and using the *Apply* button. If rotation tools are not visible, you can recall it

by pressing the *Ctrl* key of the keyboard and clicking on the *Apply* button.

4.3 Scales

Real and reciprocal lattices have their own scales. These scales can be modified by pressing the <+> and <-> keys of your keyboard or using the mouse (see 4.2.3) :

- <+>: Zoom + (∗ 1.15),
- <-> : Zoom - (/ 1.15),

or, using the functions "**Zoom ±**" and "**General Scale**" of the ***View*** Menu .

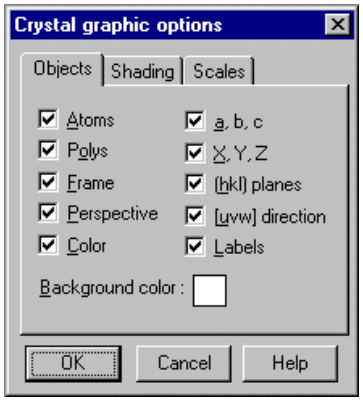
4.4 Planes translations

When the visualisation of a particular plane is asked for, CaRIne selects the plane of the (hkl) family which is closest to the lattice origin. The origin is that of the reference frame (R_m) and can therefore be visualised by displaying the reference frame (R_m). If the lattice does not have enough atoms, it is possible that none of the atoms displayed belong to this particular plane. It is then necessary either to enlarge the lattice (see ***Crystal*** Menu) or to translate the plane. The latter operation corresponds to the function : **"Translation ± of a plane"** (see ***hkl/uvw*** Menu) .

4.5 The "Graphics" command

The " **Graphics**" command (***View*** Menu) allows the graphical representation of the current crystal, the stereographic projection, the x-ray diffraction pattern or the reciprocal lattice to be modified. "**Graphics**" opens the appropriate dialogue box in accordance with the activated window :

• In the case of **crystal windows**, can be displayed separately :



• **Atoms** : The atoms (which don't belong to selected (hkl) planes).

• **Polys** : The coordination polyhedrons.

• **Frame** : The frame and links between atoms.

• **Perspective** : The perspective effect (cancel it to get a plane projection)

• **Colour** : The colour of the atoms. When off, the atoms appear transparent.

• **abc, xyz frame** : The (**a**,**b**,**c**) and (**x**,**y**,**z**) reference frames (see §4.1).

• **(hkl) planes** : The atoms which belong to the selected (hkl) plane(s) (see ***hkl/uvw*** Menu).

• **[uvw] direction** : The [uvw] direction is displayed with a red arrow (see ***hkl/uvw*** Menu).

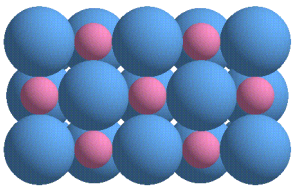
• **Labels** : Display of chemical symbol on atom, with the degree of oxidation.

• **Background colour**: Allows to change the background colour of the active window.

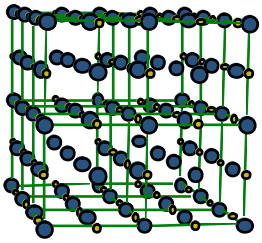
• **Shading Effect**: The shading effect is optimal with a thousands colour display.

• **Zone Size** : The value of each colour zone is given in pixels. The shading effect is better with a smaller value of the zone size, but the resulting image is larger and the computing time is larger.

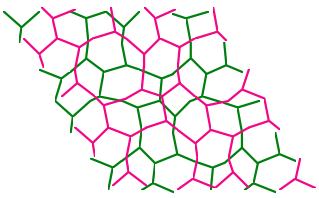
• **Dephtshading** : The intensity of the colours vary as a function of the distance between the object and the user. The maximum intensity change is given in the **Variation** box.



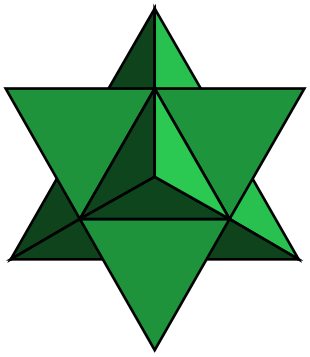
With shading



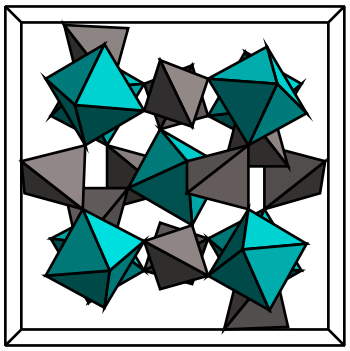
With atoms and frame



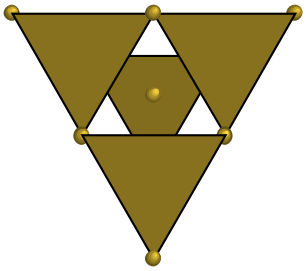
With frame only



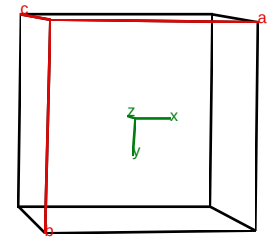
With polyhedrons and shading



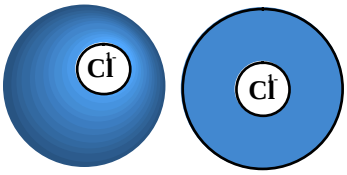
With polys, frame and shading



With polys and atoms



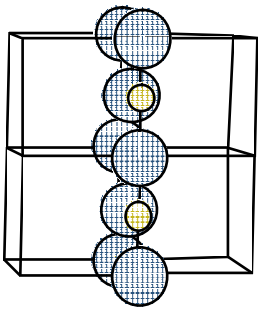
With frames and reference frames (xyz ; abc)



With shading

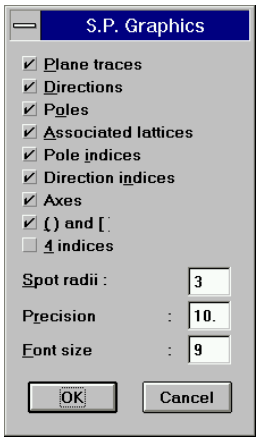
Without shading

Atoms with label

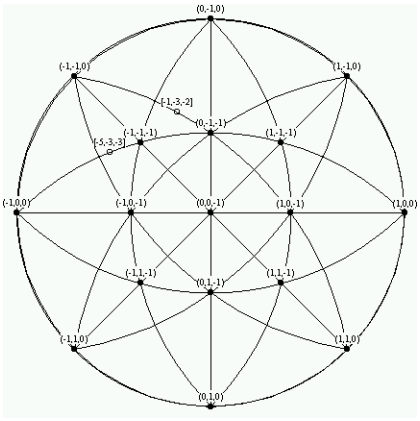


With frame and hkl plane

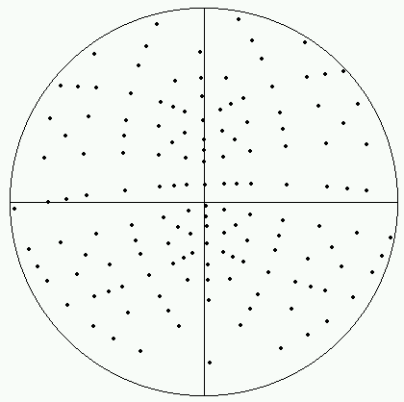
• When working in a **Stereographic Projection window**, can be displayed separately :



- **Plane traces** : The projections of the plane's traces.
- **Directions** : The projection spots of the directions.
- **Poles** : The projection spots corresponding to the poles.
- **Asso. Lattices** : The projections belonging to the associated lattices.
- **Pole indices** : The pole indices.
- **Direction indices** : The direction indices.
- **Axes** : The projection axes.
- **Spot Radii** : in pixels.
- **Drawing precision** : Each trace is composed of this number of segments.
- **Font size**.
- **4 Indices** : Cross off this box to get a four indexes output (hexagonal system).

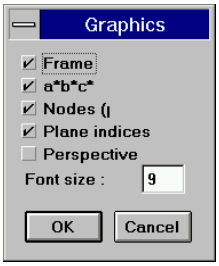


With poles, directions and traces



With axes and poles

• When working in a separately : **reciprocal lattice window**, can be displayed



• **Frame** : The frame of the reciprocal lattice.

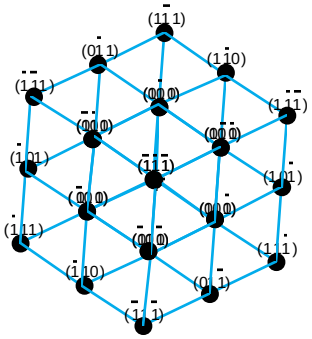
• **a*b*c*** : The reference frame.

• **Nodes** : The nodes corresponding to the planes.

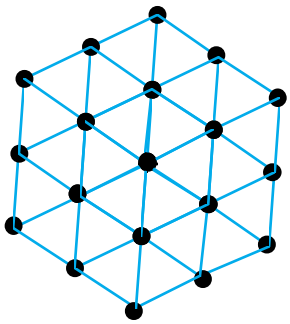
• **Plane indices**.

• **Perspective** : The perspective effect.

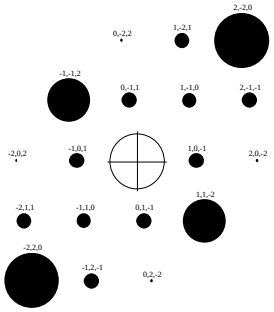
• **Font size** : The size of the characters.



With nodes, indices and frame

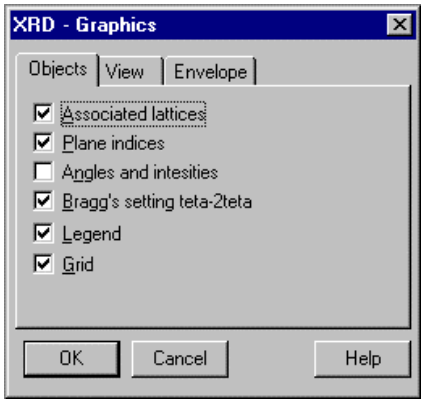


With nodes and frame



With nodes and indices

• Finally, in the case of a **XRD window**, can be displayed separately :

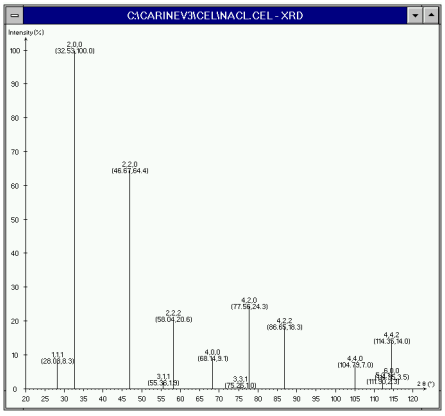


- **Associated Lattices** : Superposition of the associated lattice XRD diagrams.
- **Plane indices** : The planes indices.
- **Angle and Intensity** : The diffraction angle with the relative intensity.
- **Bragg Figure** : The Bragg's geometry drawing.
- **Legend** : The list of crystals which the XRD diagrams are calculated.
- **Grid**.

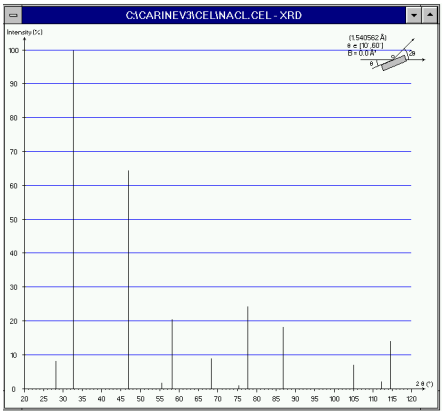
- **2θ1, 2θ2** : These two values give the angle window in which the XRD diagrams are displayed.
- **% mini** : Minimun intensity for the peaks to be indexed.

Also, the XRD diagrams can be displayed with different options (see Chap 7) :

1) as a list of peaks
2) as an intensity versus angle function (squared Cauchy function with one parameter : the integral peak width β).
3) both 1/ and 2/



With indices, angles and relative intensities



With grid and Bragg's figure

CHAPTER 5
Lattice Associations

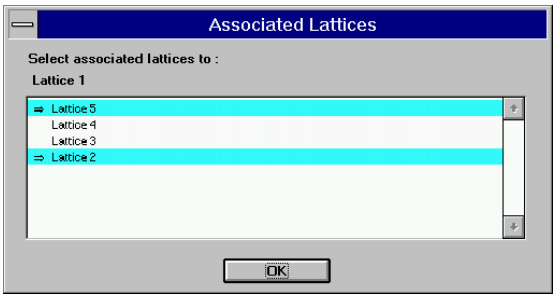
5

Any lattice can be associated with another one, in order to study the relations of orientation between matrixes and precipitates or substrate and film, for example. The association of lattices can be completed with a condition of orientation between the different lattices (Relation of Epitaxy).

5.1 "Matrix - Precipitate" type association

If one wishes to associate lattices without giving them a condition of orientation, a matrix should be chosen (current lattice), then the command "**Associated Lattices**" of the Menu ***Specials***.

The following dialogue box appears :



The precipitates should then be chosen from the list of lattices which are opened.

To select or unselect a lattice click on its name. Here the precipitates are *Lattice 2* and *Lattice 5*; the matrix being *Lattice 1*.

If one wishes the precipitates to keep their orientation in relation to the matrix (during rotations and projections), cross off the box ☒ **Apply the rotations to the associated Lattices** of the matrix (function " **Rotations**" Menu ***View***).

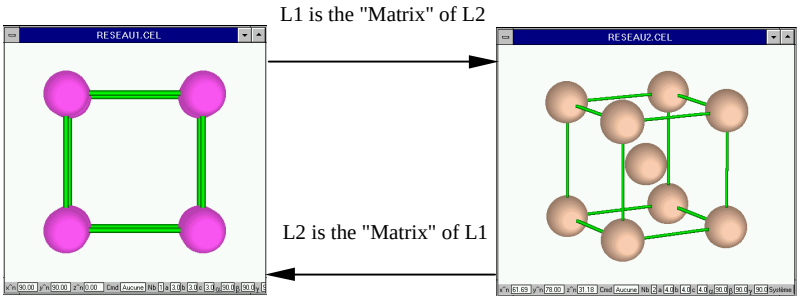
> Warning : The rotation of a precipitate does not bring about that of the matrix.

In front of each lattice there is a symbol showing the type of association :

⇒ : Matrix-Precipitate association (Matrix ⇒ Precipitate)
⇐ : Matrix-Precipitate association (Precipitate ⇐ Matrix)
⇔ : Crossed Matrix-Precipitate association.

The number of precipitates is unlimited, and it is possible to work simultaneously with several groups of associated lattices.

Crossed Association



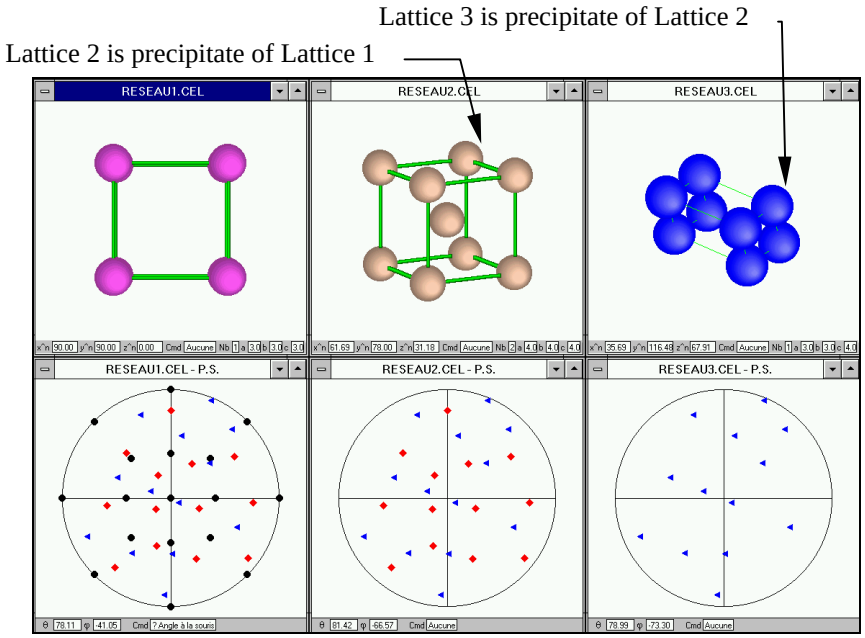
F5.1 : Crossed association.

CaRIne allows crossed associations to be made between several lattices

(see fig F5.1). In this way, a lattice L_1 can be the "matrix" of a lattice L_2 and this same lattice L_2 can be the "matrix" of L_1. In order to keep the orientation of L_1 in relation to L_2, while projecting or rotating each of the two lattices L_1 and L_2 indiscriminately, cross off the ☒ **Apply the rotations to the associated Lattices** box for each of the lattices L_1 and L_2.

Stereographic Projection, XRD and "Matrix-Precipitate" type association

- The stereographic projection (S.P.) of a matrix M with n precipitates is the superposition of the stereographic projections of the matrix M and these of its precipitates $P_{1..n}$. If the precipitates $P_{1..n}$ are also the matrixes $M_{1..n}$ of other precipitates $P'_{1..n}$, then the S.P. will also be the superposition of the stereographic projections of the precipitates $P'_{1..n}$ etc... (see fig. F5.2).



F5.2 : Superposition of stereographic projections

As fig. F5.2 illustrates :

- the stereographic projection of lattice 1 is the superposition of the stereographic projections of the lattices 1,2 and 3;
- that of lattice 2 is the superposition of the stereographic projections of the lattices 2 and 3;
- that of lattice 3 is the stereographic projection of the lattice 3 only.

Note : When several stereographic projections are superimposed, the projection parameters of each lattice must be set separately, by activating the lattice's windows one by one , then by using the function "**Parameters**" Menu ***Special/Stereo.Proj***. (see Chap.6 §6.2).

- The X-Ray diffraction pattern of a matrix M of n precipitates is the superposition of the X-Ray diffraction patterns of the matrix M and those of its precipitates $P_{1..n}$.

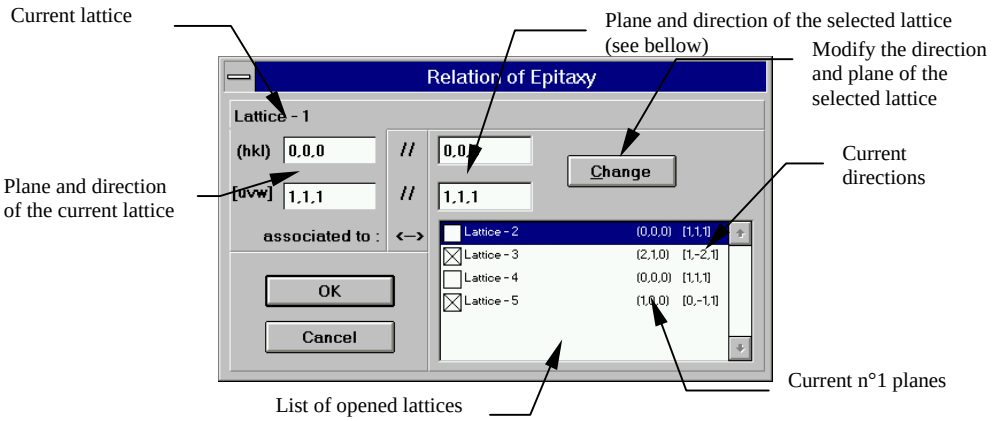
  In the case of the associative schema of figure F5.2 :

  - XRD diagram of the lattice 1 is the superimposition of the XRD diagrams of lattices 1 and 2;
  - that of the lattice 2 is the superimposition of the XRD diagrams of lattices 2 and 3;
  - that of the lattice 3 is the XRD diagram of lattice 3 only.

  When several x-ray diagrams are superimposed, it is possible to give a proportion to each phase (see Chap. 7).

5.2 Association with "Relation of Epitaxy"

When you wish to associate lattices by giving them conditions of orientation, ask for the command " **Relations of Epitaxy** " of the Menu ***Specials***. the following dialogue box will appear :



The lattices to be associated with the current lattice should be chosen from the list of the opened lattices.
To select or unselect a lattice, click on its name. In order for it to be associated with the current lattice, cross off the check box which is to the left of the name (click on a second time to associate or disassociate). To modify the plane and direction of epitaxy of the selected lattice, press Change.
In the example of figure F5.3, the associated lattices are : *Lattice 1*, *Lattice 3* and *Lattice 5*.

CaRIne automatically associates the lattices of the relation of epitaxy by a relation of crossed matrix-precipitate type. Furthermore, to keep the conditions of orientation due to the relation of epitaxy, CaRIne automatically crosses off the check box ☒ **Apply the rotations to the associated Lattices** of each of the lattices of this relation.

The number of lattices associated by a relation epitaxy is unlimited.

Warning : Condition of parallelism : A relation of epitaxy between several lattices should be given in such a way that all planes are parallel to each other and all directions parallel to one another. However, it is possible to orient a group of lattices by several relations of epitaxy and to keep these conditions of orientation (see § 5.3 Orienting a group of lattices by giving several relations of epitaxy).

Example :

Lattice 1		Lattice 3		Lattice 5
$h_1k_1l_1$	//	$h_3k_3l_3$	//	$h_5k_5l_5$
$u_1v_1w_1$	//	$u_3v_3w_3$	//	$u_5v_5w_5$

When the modifications are validated by the button [OK], CaRIne puts the lattices associated in position of epitaxy if and only if :

- all the planes are different from the plane (000),
- all the directions are different from the direction [000],
- for all the associated lattices, the direction is comprised within the plane.

Stereographic Projection, XRD and "Relation of epitaxy" type association

The stereographic projection (or the diagram of x-ray diffraction) of a lattice which has relations of epitaxy with other lattices is the superimposition of the stereographic projections (or the x-ray diffraction patterns) of this lattice and those of its associated lattices.

5.3 Orientating a group of lattices by giving several relations of epitaxy

By using several times the function " **Relation of Epitaxy** ", a group of lattices can be orientated by several relations of epitaxy which do not comply with the condition of parallelism of the previous paragraph.

Example : To orientate 3 cubic lattices by the 2 following relations of epitaxy :

Relation 1		
Cubic 1		Cubic 2
(111)	//	(110)
[-1-12]	//	[1-10]

Relation 2		
Cubic 1		Cubic 3
(100)	//	(102)
[0-10]	//	[2-2-1]

Once these 3 cubic lattices have been created,

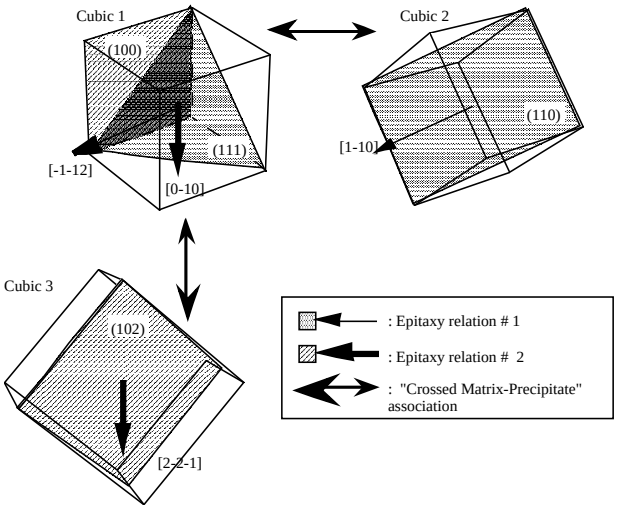
⇒ select the cubic 1 window,
⇒ ask for the function "**Relation of Epitaxy**",
⇒ enter the plane (111) and the direction [-1-12] for cubic 1,
⇒ select cubic 2 from the list of opened lattices, then enter the plane (110) and the direction [1-10], press Change,
⇒ press OK.

The cubic lattices 1 and 2 are in position of epitaxy and are linked by an association of the type "crossed matrix-precipitate".

⇒ select the cubic 3 window,
⇒ ask for the function "**Relation of Epitaxy**",
⇒ enter the plane (102) and the direction [2-2-1] for cubic 3,
⇒ select cubic 1 from the list of opened lattices, then enter the plane (100) and the direction [0-10], press Change,
⇒ press OK.

The cubic lattices 1 and 2 are in position of epitaxy and are linked by an association of the type "crossed matrix-precipitate". The cubic lattice 2 has followed the rotation of the cubic lattice 1.

Finally, the following associative schema is obtained :



F5.3 : Two relations of epitaxy.

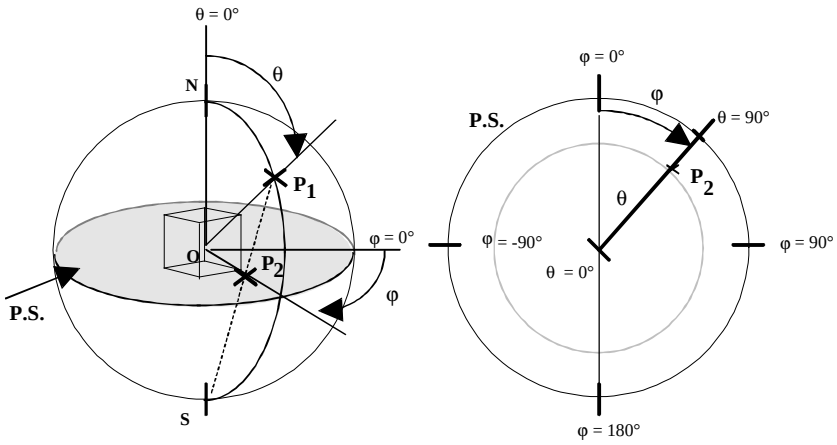
CHAPTER 6
The stereographic projections

6

CaRIne computes, displays and let you interact with the stereographic projections of all structures.

6.1 Introduction

The stereographic projections are used to display the symmetries of the external crystal faces and of the internal structure. It can also be used to orient a crystal.



F6.1 : Stereographic projection with the geometric conventions used by CaRIne.

Consider a sphere surrounding a crystal. From the centre O of the crystal and of the sphere, we can trace the normal to a (hkl) plane. This line intersects the sphere in P_1. This point is called a "pole". This pole can be located with θ and φ angles, as given on F6.1. P_1 is projected on the equatorial plane, by drawing a line between P_1 and S. P_2 is the intersection of (P_1, S) and the equatorial plane. P_2 is the stereographic projection of the pole P_1. The disk P.S. is called the stereographic projection.

We can also build the projection of the intersection of an (hkl) plane with the sphere. To do this, we would choose the (hkl) plane which comprised the point o. The intersection of this plane with the sphere is a circle. CaRIne will then project the part of this circle which is located in the North hemisphere.

The third kind of objects which can be projected are the directions. The principle is the same as for a pole.

Remark : Only the objects of the North hemisphere are projected on the stereographic projection.

Notations : For brevity reasons, we will often call "pole (hkl)" the "stereographic projection of an (hkl) pole" (same for traces and directions).

6.2 Menu *Specials/Stereo.Proj.*

This menu allows the creation and the use of stereographic projections.

Create

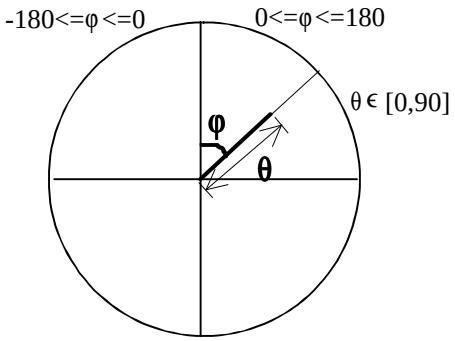
This function creates a new window in order to display the stereographic projection of the active crystal. The window title recalls the name of the crystal followed by the "S.P." mention (Stereographic Projection).

The orientation of the stereographic projection corresponds to the crystal orientation, then projections and rotations will have an effect on both the crystal and its stereographic projection.

The stereographic projection can be copied in the clipboard (WMF format, see Menu ***Edit***). It is also possible to directly print it or save the image in a file (see Menu ***Files***).

Use of the protractor :

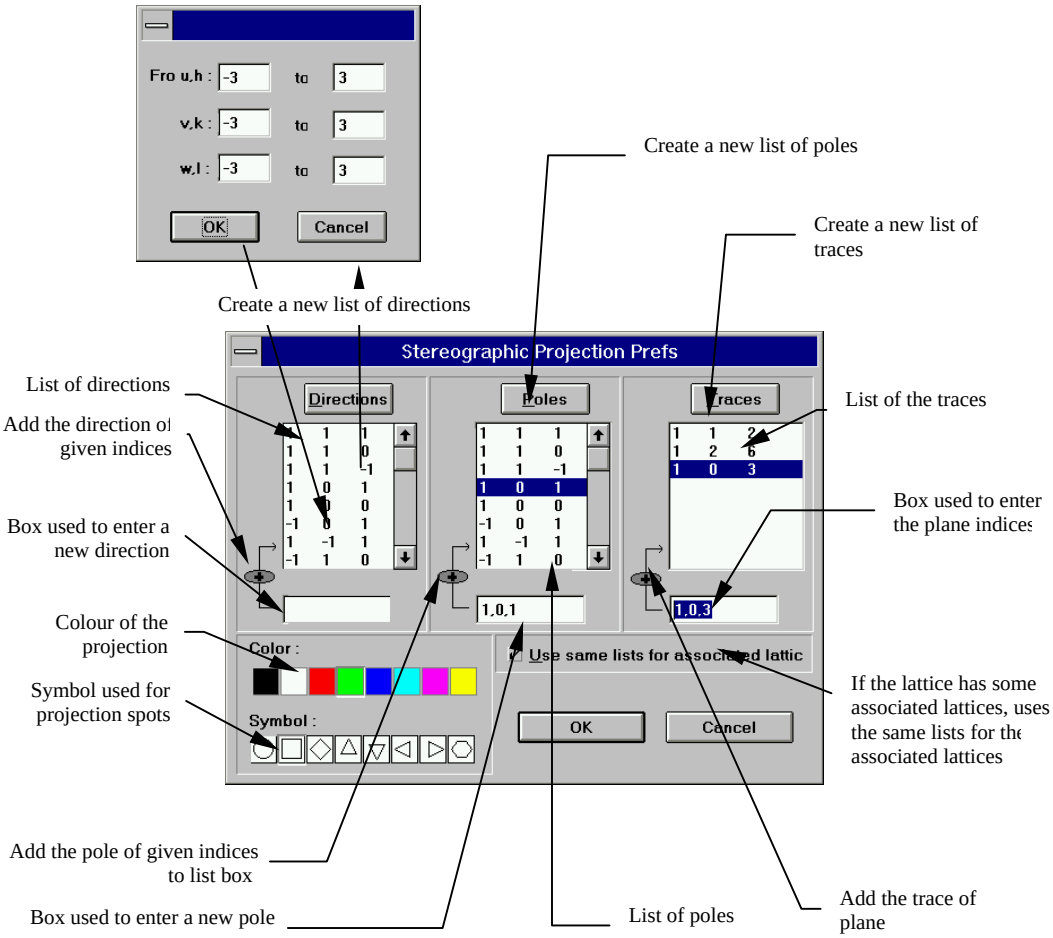
Each stereographic projections has a protractor. It is represented by a cursor which is active when the mouse is located inside the S.P. circle. The θ, φ coordinates are given in the information bar (bottom of the window).



Parameters

This function is used to build the list of objects to display on the stereographic projection. The objects are the projection spots of directions, poles and the projections of plane's traces. With this function, the user can also modify the symbol and colour of the projection spots.

Spots corresponding to directions will be displayed with " empty" symbols, whereas spots corresponding to poles will be " full" symbols. If the current lattice has some associated lattices, the stereographic projection will be the superposition of the projections of all the lattices. You can choose to use the same directions, poles and traces lists for the associated lattices, just by clicking in " ☒ **Use same lists for associated lattices**".


Fro u,h : -3 to 3
v,k : -3 to 3
w,l : -3 to 3
OK
Cancel
Create a new list of directions
Create a new list of poles
Create a new list of traces
Stereographic Projection Prefs
Directions
Poles
Traces
List of directions
Add the direction of given indices
Box used to enter a new direction
Colour of the projection
Symbol used for projection spots
List of the traces
Box used to enter the plane indices
1,0,1
1,0,3
Color :
Symbol :
Use same lists for associated lattic
If the lattice has some associated lattices, uses the same lists for the associated lattices
OK
Cancel
Add the pole of given indices to list box
Box used to enter a new pole
List of poles
Add the trace of plane

The direction list, pole list, trace of plane list can be loaded and saved from/to text files (click on a list box with the right button to select one of these functions). Also CaRIne generates the plane form from the entry of 3 indices. For example, you can create the (110), (-210), (1-20) list from the entry of (110) in the hexagonal system.

A double-click in the stereographic projection (but outside the projection disk) will also open the "parameters" dialogue box.

You will find in Appendix D a description concerning the use of the lists.

Export to ASCII file

Use the function *Special/Stereographic projection/export to an ASCII file* to export the pole and direction projections polar coordinates (θ ϕ) into a text file.

Example :

CaRIne Crystallography 3.1

Format : (h,k,l) (or [u,v,w]) teta(°) phi(°)

FCC

Poles

(-1,-1,-1)	*54.74*	*-45.00*
(1,1,0)	*90.00*	*-45.00*
(1,1,-1)	*54.74*	*135.00*
(-1,0,-1)	*45.00*	*-90.00*
(1,0,0)	*90.00*	*-90.00*

? [uvw] with mouse

Active this function using the function found in the ***hkl/uvw*** Menu or using the corresponding stereographic projection tool. Then, click inside the projection circle and CaRIne will answer with the closest [uvw] spot. These u,v,w indexes will be chosen in the range set with the function "**Spread of research**".

? (hkl) with mouse

Same as previous function, for the (hkl) pole projections.

Spread of search

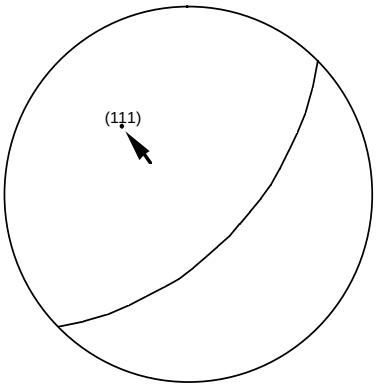
This function allows the user to modify the range of u,v,w and h,k,l indexes when searching for a direction or pole projection in the vicinity of the mouse location (see functions " **? (hkl) with mouse**" and " **? [uvw] with mouse**").

? Angle with mouse

This function gives the angle between poles and/or directions projections. Simply select two poles, two directions, or one pole and one direction with the mouse. CaRIne will answer with a dialogue box which recall the indexes of the selected spots and the angle between them.

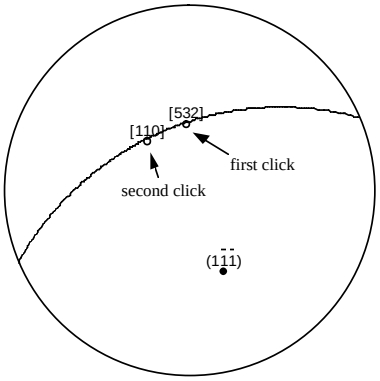
? Trace from 1 pole

You can add or remove a trace just by selecting the corresponding pole with the mouse. It is then very easy to see which spots form a 90° angle with a specific pole.



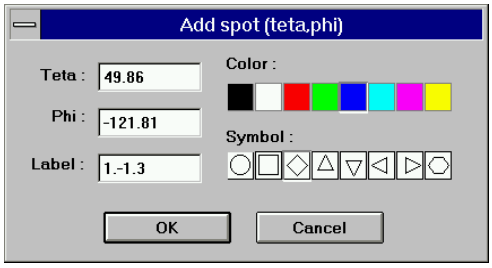
? Trace from 2 zones

This function is used to display or not display the trace of a specific (hkl) plane, from the selection of two directions using the mouse. These two directions belong to the plane.



Add Spot (teta, phi)

With this function, you will place spots at given (teta,phi) position. Each specific spot has a colour, a symbol and a label. If you enter h,k and l values as a label (using periods to separate values) CaRIne will display it with an (hkl) format. Remark that you don't have to give h,k,l indices, all kinds of text being a possible label.



To add a fixed spot, follow this sequence :

⇒ select "**Add Spot (teta, phi)**" function,
⇒ place the mouse to the desired location where you want to place a spot and click on,

⇒ CaRIne displays a dialogue box and asks to enter a label and to choose a colour and a symbol. You can change the teta and phi values. Press on [OK].

Remark : If you know the teta and phi values, you can click any position on the stereographic projection and just give the teta and phi values in the dialogue box.

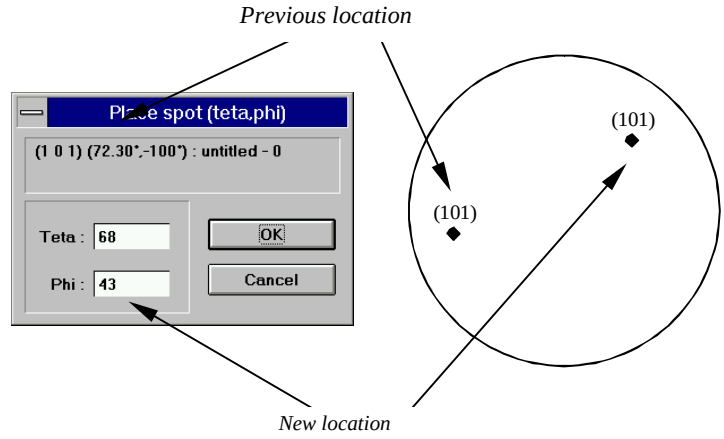
This spot will remain immobile. Rotating the crystal or asking for specific projections will have no effect on its location.

Remove Spot

Just click as closed as possible to a spot to remove it.

Move Spot to (teta, phi)

This function allows the user to orient the stereographic projection and its respective real lattice. The first step is to display the spot that we want to place on the projection (pole or direction). Then, select the function "**Move Spot to (teta, phi)** " and click on the pole (or direction) spot. CaRIne answers with the following dialogue box :



You can then enter the new values for teta and phi.

Set Plane n°1 From Spot

This function allows to define the plane number 1 (see Chap.2 Menu ***hkl/uvw***) from the selection of a pole with the mouse. If you have asked for the visualisation of planes (function " **Graphics**" linked to the real lattice), you will see the new plane #1 being actualised.

Set [uvw] From Spot

This function is similar to the previous one. It allows to define the current direction [uvw] (see Chap.2 Menu ***hkl/uvw***) from the selection on the stereographic projection. This can be used, for example, to define the direction around which the rotations are done (see Rotation around [uvw]), or to do a projection // [uvw] (see Menu **(hkl)/[uvw]**).

Show Spot(teta,phi)

The function *Special|Stereo Proj|Display (q,f)* allows to display the (q,f) for a specific pole or direction. Simply select this function and click on a specific spot.

6.3 Orientate the stereographic projection

The sterographic projections can be orientated using different ways :

• Rotations around a [uvw] direction : CaRIne will use the current direction of the crystal. This direction can be defined by selecting two atoms with the mouse (see function " **? [uvw] with mouse** " Menu ***hkl/uvw***), by the indices (see function "**Choice of [uvw]**" Menu ***hkl/uvw***) or by clicking on the stereographic projection (see function " **Set [uvw] from spot**" Menu ***Stereo.Proj.***).

• Rotations around a (hkl) pole : CaRIne will use the plane #1 of the crystal (Menu ***hkl/uvw***). This plane can also be defined using the function "**Set (hkl) from spot**".

• Move a pole or a direction spot to a specific position :

⇒ functions " **Projection // [uvw]** " or " **Projection Perp. (hkl)** " (Menu ***hkl/uvw***) (place the current direction or plane at the centre of the projection).

⇒ function "**Move spot to (teta, phi)**" (see §6.2).

⇒ using the mouse :
To move a spot on the stereographic projection, press the *Ctrl* key of the keyboard and click on a specific spot, and move the mouse.

To move the stereographic projection around a spot (i.e. rotate the crystal around a direction or a pole), press the *Ctrl* Key of the keyboard, then select a spot with a double-click. A symbol appears to show that this spot is now fixed (⏚). You can now move the stereographic projection as explained before. Perform another double-click on the fixed spot (⏚) in order to free it.

This function allows to use the stereographic projection as an easy tool to orientate the crystal and also the reciprocal lattice.

6.4 Menu *View*

Graphics Ctrl-G

This function opens the dialogue box dedicated to the graphic options relative to the stereographic projection. It is possible to display the poles, directions or plane traces separately or together. This option also allows you to modify the font size (see Chap.4).

CHAPTER 7

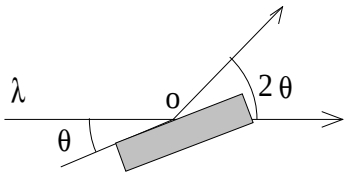
The X-Rays diffraction patterns for random orientated powders

7

CaRIne computes the positions and intensities of the X-Rays diffraction peaks from the knowledge of the unit cell.

7.1 Introduction : Calculation of peak intensities

The calculation of the X-Rays diffraction is done from the unit cell, for a random orientated powder, and with the Bragg configuration as shown below :



F7.1 :Bragg's geometric configuration.

The θ angle is called **Bragg angle**.

The diffraction angle is calculated from the interplanar distance and from the incident wave length λ :

$$\lambda = 2 \cdot \left(\frac{d_{hkl}}{n} \right) \sin\theta \qquad \text{(E7.1)}$$

For each (hkl) plane, the **structure factor** is computed using equation E7.2 :

$$F_{hkl} = \sum_{n=1}^{N} f_n \cdot f_{occ} \cdot e^{2\pi i (h.x_n + k.y_n + l.z_n)} \qquad \text{(E7.2)}$$

where f_n is the **atomic scattering factor** for x-rays; x_n, y_n et z_n are the coordinates of the n $\underline{th}$ atom of the cell; f_{occ} is the occupation factor of the site ($0 \leq f_{occ} \leq 1$).

The atomic scattering factors vary as a function of the Bragg angle and the x-ray wave length.

CaRIne uses the following approximation :

$$f\left(\frac{\sin\theta}{\lambda} \right) = \sum_{i=1}^{4} a_i . e^{-b_i \cdot \left(\frac{\sin\theta}{\lambda} \right)^2} + c \qquad \text{(E7.3)}$$

where a_i, b_i et c are fitting coefficients. The list of the different ions which are differentiated is given in Appendix C.

To compute the peak intensities, CaRIne takes into account the following factors :

- the **Lorentz factor** :

$$f_{Lorentz} = \frac{1}{4 . \sin^2\theta . \cos\theta} \qquad \text{(E7.4)}$$

- the **polarisation factor** :

$$f_{Polarisation} = \frac{1}{2} \cdot \left(1 + \cos^2\theta \right) \qquad \text{(E7.5)}$$

- the **temperature factor** (supposed to be constant for all atoms of the cell) :

$$f_{Temperature} = e^{-2.B.\left(\frac{\sin\theta}{\lambda}\right)^2} \qquad \text{(E7.6)}$$

Remark : the temperature factor is given by the user.

- the **multiplicity factor**, which depends on the (hkl) plane and on the unit cell.

Finally, the intensities of the peaks are computed as :

$$I = \frac{\|F\|^2 \cdot \left(\frac{1+\cos^2 2\theta}{\sin^2\theta \cdot \cos\theta}\right) \cdot e^{-2B\left(\frac{\sin\theta}{\lambda}\right)^2} \cdot p}{V} \qquad \text{(E7.7)}$$

where V is the unit cell volume.

And these intensities are normalised relatively to the highest peak.

Remark : the absorption factor is not taken into account in the computation of the normalised intensities because this factor is independent of θ :

$$f_{Absorption} = \frac{1}{2\mu} \qquad \text{(E7.8)}$$

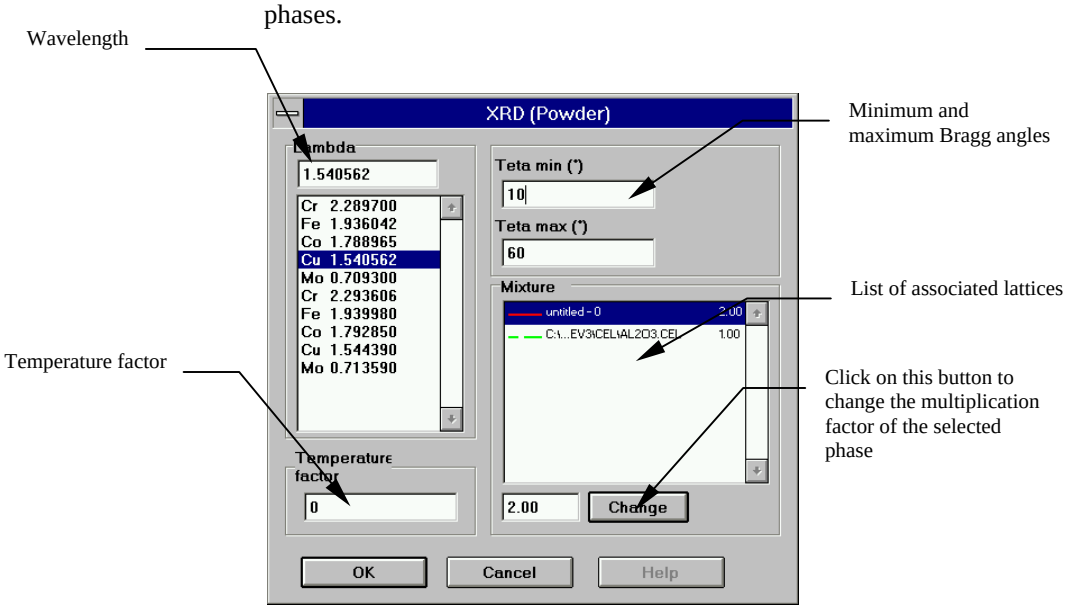
But this should be remembered when doing powder mixing, and the user should enter this factor in the proportion coefficient for each phase (see function "**Create**" §7.2).

Create

This function computes the powder-XRD of the current crystal.

A dialogue box appears, in which the different parameters can be set up. Then, you have to choose :

- ⇒ the wavelength of the X-Rays (you can either enter a value or click on one of the proposed ones),
- ⇒ the minimum and maximum Bragg angles ,
- ⇒ the temperature factor,
- ⇒ in the case of existence of associated lattices to the current crystal, these lattices appear in the "Mixture" box. After selecting one of these using the mouse (simple-click), you can change its multiplication factor (2.00 in our example). The calculated intensities will be multiplied by this factor, and then, normalised to the most intense peak of all present phases.



A double-click on a phase name in the "mixture" box allows to access to the graphic parameters (colour and motif of the lines). This is equivalent to the "**Preferences**" function (see below).

After this set-up, you can click on [OK]. CaRIne creates a new window in order to display the X-Rays diffraction diagram. The title of this window recall the name of the real lattice with the mention "XRD (powder)".

The diagram can be copied (Menu ***Edit***), printed (Menu ***Files***) or saved on disk as a picture (Menu ***Files***).

A double-click inside the XRD window re-opens the parameters dialog box.

Note :
If one wants to change the mixture coefficients without recalculation of the XRD pattern, the Mixture function should be used (see page 7-6).

Preferences

This function gives a colour and a motif to the diagram corresponding to the real lattice active window. Initially, all diagrams are drawn in black with solid lines.

Save XRD as ASCII File

This function allows to save the XRD diagram calculated by CaRIne as an ASCII file.

Example :

CaRIne Crystallography 3.0
C:\CARINEV3\CEL\CL\NACL.CEL
Max. value : 429664.312

Number of peaks : 15

(hkl)	2teta	intensity	dhkl	fs^2	P
(200)	32.53	100.0	2.750	6305.23	3
(400)	68.14	6.1	1.375	1990.76	3
(600)	114.35	1.2	0.917	571.18	3
(420)	77.56	14.3	1.230	1500.08	12
(220)	46.67	56.4	1.945	3958.81	6
(440)	104.79	2.8	0.972	715.92	6
(531)	111.90	0.8	0.930	48.93	24
(511)	93.39	0.4	1.058	56.34	12
(331)	75.25	0.6	1.262	61.11	12
(311)	55.36	1.5	1.658	76.72	12
(111)	28.08	8.6	3.175	296.54	4
(442)	114.35	4.9	0.917	571.18	12
(422)	86.65	9.5	1.123	1156.04	12
(222)	58.04	15.8	1.588	2733.14	4
(333)	93.39	0.1	1.058	56.34	4

Mixture

This function allows the user to affect a coefficient to every phase for diffraction pattern of a powder mixture.

Import Exp. File

This function allows the user to import its own experimental data file. This file (ASCII File) should respect the following format :

- first line (header) : **XRD Exp. File**,
- the second line gives the number of values in the file,
- then, the file is a succession of lines with two values separated with "spaces" or "TAB". The first value of each line is the diffraction angle (°) . The second value is the intensity.

Example :

```
XRD EXP. File
209
8.0000      38.50
8.2500      34.50
8.5000      36.25
8.7500      35.25
9.0000      42.50
9.2500      43.25
9.5000      32.50...
```

Prefs. Exp. File

This function allows to change the colour and motif of the experimental diagram (see previous function). Initially, these options are set to black and solid lines.

Remove Exp. File

This function allows to remove the experimental diagram (see previous functions).

Import Ref. File

This function allows the user to import its own reference datafile (ASTM, JCPDS, ...) . This file (ASCII file) should respect the following format :

- first line (header) : **XRD Ref. File**,
- the second line gives the **number of peaks** in the file,
- then, the file is a succession of lines with 5 values separated with "spaces" or "TAB". The first value of each line is the **interplanar distance** . The second value is the **intensity**.

These intensities should be normalised in order that the highest intensity is 100. And the three last values are the **indexes of the hkl plane**.

Example :

XRD Ref. file
60

6.583	34	1	0	0
3.800	35	1	1	0
3.293	100	2	0	0
2.660	99	2	0	0
2.489	93	2	1	0
2.31	9	1	1	1
2.1939	10	3	0	0
2.1797	31	2	0	1

etc...

Prefs. Ref. File

This function allows to change the colour and motif of the reference diagram (see previous function). Initially, these options are set to black and solid lines.

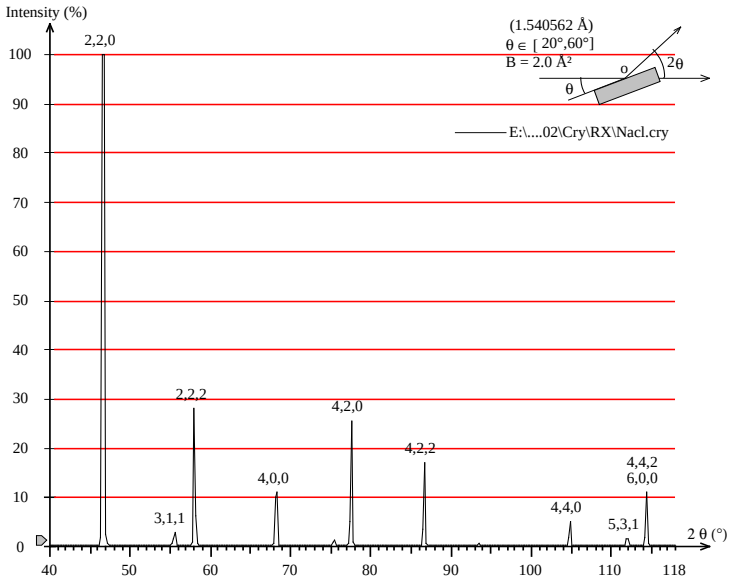
Remove Ref. File

This function allows to remove the reference diagram (see previous functions).

7.3 Menu *View*

Graphics Ctrl-G

This function allows the graphic objects to be selected independently : X-Rays diffraction diagrams of associated lattices, plane indices, angle and intensity of each peak, grid, envelopes…



The XRD diagrams can be displayed with different options :

1) as a list of peaks,
2) as an intensity versus angle function (squared Cauchy function with one parameter : the integral peak width β)
3) both 1/ and 2/

Option 2 allows the summation of several diagrams when using the association of lattices (mixture of powders).

Note :

Squared-Cauchy function : $I(x) = \frac{Imax}{\left(1 + k \cdot x^2\right)^2}$

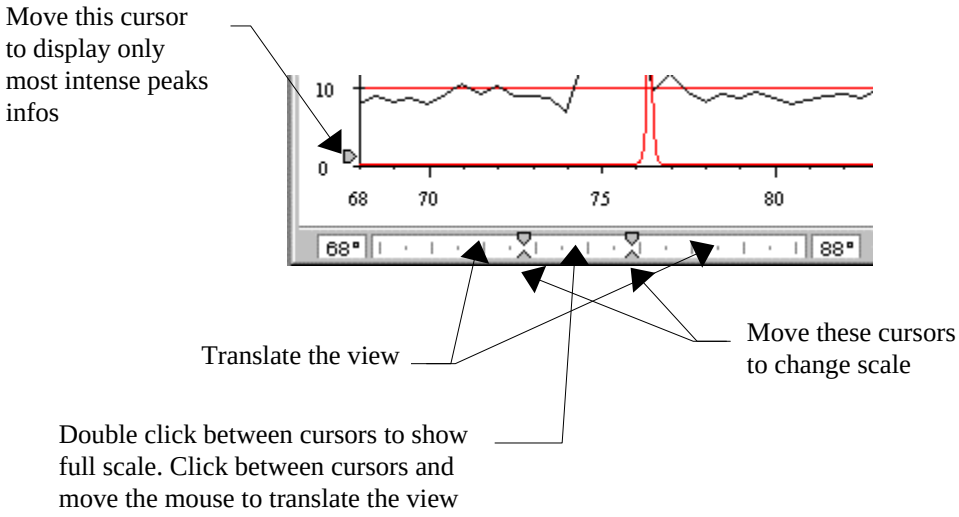
The integral width is given as : $\beta = \frac{\pi}{2\sqrt{k}}$

Then CaRIne computes k as : $k = \left(\frac{\pi}{2 \cdot \beta}\right)^2$

The FWHM (full width at half maximum intensity) is given by : $l = \frac{2\sqrt{\sqrt{2} - 1}}{\sqrt{k}}$

Change XRD scales with the mouse :

Cursors under the Bragg angle axis can be moved with the mouse in order to perform zooms. A double-click between cursors in the info-bar gets back to the original teta range (full scale). Another new function permits to display only most intense peaks infos (θ, intensity, indices). To do so, simply move the cursor with the mouse, on the intensity axis.



CHAPTER 8
The Reciprocal Lattices

8

CaRIne build and visualises the reciprocal lattice from the direct lattice.

8.1 Introduction

The reciprocal lattice is defined from the direct lattice vectors, as :

$$\mathbf{a^*} = \frac{\mathbf{b} \wedge \mathbf{c}}{\mathbf{V}}, \ \mathbf{b^*} = \frac{\mathbf{c} \wedge \mathbf{a}}{V}, \ \mathbf{c^*} = \frac{\mathbf{a} \wedge \mathbf{b}}{V}$$

where V is the cell volume, V = $\mathbf{a} \cdot (\mathbf{b} \wedge \mathbf{c})$.

The parallelepiped built on **a***,**b***,**c*** is called the unit cell of the reciprocal lattice.

For each plane of the direct lattice corresponds a node of the reciprocal lattice. For each planes' family only in the direct lattice corresponds to an infinity of reciprocal lattice points, aligned on a direction normal to the planes.

The direct and reciprocal lattices are conjug ated and have the same point symmetry. But their space groups are generally differents.

In the CaRIne software, the relative orientation of **a**, **b**, **c** and of **a***, **b***, **c*** vectors is always respected. Rotating the direct lattice will then induce the corresponding rotation of the reciprocal lattice. As for the real lattice

you can use the «intuitive rotations» with the mouse (see §4.2.3). General scale and radii scale can also be modified using this way.

The norms of the **a***, **b***, **c*** vectors will also be automatically computed as soon as the vectors **a**, **b**, **c** are modified. Nevertheless, the reciprocal lattice scale allows the zoom in/out of each lattice independently (see Chap.4 §4.3).

In the reciprocal lattice, a family of (hkl) planes is represented by a node M such as :

$$\mathbf{d}^*_{hkl} = \mathbf{OM}^* = h.\mathbf{a}^* + k.\mathbf{b}^* + l.\mathbf{c}^*$$

So, a vector $\mathbf{d}^*_{hkl}$ of the reciprocal lattice represents the orientation of the planes' family in the crystal ($\mathbf{d}^*_{hkl} \perp (hkl)$) and the interplanar distance ($\mathbf{d}_{hkl} = \frac{1}{\|\mathbf{d}^*_{hkl}\|}$). CaRIne allows to take angles and distances in the reciprocal lattice, using the mouse.

As for the direct lattice (see Chap.1 §1.4), it is possible to work in two dimensions in the reciprocal lattice :

1/ first, of all one can show (h k 0) nodes by using the " **Spread of...** " function (see Chap. 8.2). It is then possible to do a projection perpendicular to the (001) plane.

2/ second, by one can visualise a "cut" of the reciprocal lattice, perpendicularly to a [uvw] zone axis (see Chap. 8.2, function " **Zone axis**"). This function can be very useful for electron diffraction pattern analyses.

Structure factor calculations :

When CaRIne build the reciprocal lattice, the structure factors are computed for each (hkl) family, with the atomic scattering factors taken as f = Z (electron number, taking into account the oxidation level). In the case of no chemical symbol name has been assigned to atoms, the "f"

factors are set to "1". In this case, the spheres of the real lattice can be considered as lattice points.

If the structure factor F_{hkl} is different from "0", a node for hkl will be shown in the reciprocal lattice.

$$F_{hkl} = \sum_{n=1}^{N}{}' f_n \cdot e^{2\pi i(h \cdot x_n + k \cdot y_n + l \cdot z_n)}$$

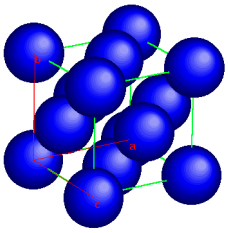
where x_n, y_n, z_n represent the position of the n $\underline{\text{th}}$ atom in an elementary cell of N atoms.

The origin (0,0,0) of the reciprocal lattice is shown by a cross-centred circle (⊕).

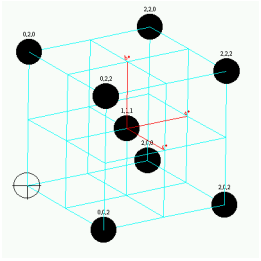
Example :

The face-centred cubic real lattice produces a body-centred cubic reciprocal lattice :

1/ Select " **Cubic**" and " **Face-centred (F)** " in the Menu ***Cell*** (do not give names to atoms)
2/ create the reciprocal lattice, with h,k,l between 0 and 2.



⇒



FCC real lattice

Reciprocal lattice

Some geometric relationships :

- The Weiss zone axis law :

  If (hkl) belongs to the [uvw] zone, then $\mathbf{d}^*_{hkl} \cdot \mathbf{d}_{uvw} = 0$

- Relations between the direct lattice vectors and the reciprocal lattice vectors :

  $\mathbf{c}^* \cdot \mathbf{a} = 0$ $\quad$ $\mathbf{c}^* \cdot \mathbf{b} = 0$
  $\mathbf{a}^* \cdot \mathbf{b} = 0$ $\quad$ $\mathbf{a}^* \cdot \mathbf{c} = 0$
  $\mathbf{b}^* \cdot \mathbf{c} = 0$ $\quad$ $\mathbf{b}^* \cdot \mathbf{a} = 0$

- The addition rule :

$$\mathbf{d}^*_{h_1+h_2,k_1+k_2,l_1+l_2} = \mathbf{d}^*_{h_1k_1l_1} + \mathbf{d}^*_{h_2k_2l_2}$$

- The zone axis of two planes :

$$\mathbf{d}_{uvw} = \mathbf{d}^*_{h_1k_1l_1} \wedge \mathbf{d}^*_{h_2k_2l_2}$$

  i.e. : $u = k_1l_2 - k_2l_1$
  $v = l_1h_2 - l_2k_1$
  $w = h_1k_2 - h_2k_1$

- The plane containing two directions :

$$\mathbf{d}^*_{hkl} = \mathbf{d}_{u1v1w1} \wedge \mathbf{d}_{u2v2w2}$$

  i.e. : $h = v_1w_2 - v_2w_1$
  $k = w_1u_2 - w_2v_1$
  $l = u_1v_2 - u_2v_1$

- The interplanar distance :

$$\frac{1}{\mathbf{d}_{hkl}} = \left\| \mathbf{d}^{*}_{hkl} \right\|$$

- The normal to a plane :

$$\mathbf{n}_{hkl} = \frac{\mathbf{d}^{*}_{hkl}}{\left\| \mathbf{d}_{hkl} \right\|}$$

- The angle between two normals :

$$\cos\theta = \frac{\mathbf{d}^{*}_{h1k1l1} \bullet \mathbf{d}^{*}_{h2k2l2}}{\left\| \mathbf{d}^{*}_{h1k1l1} \right\| \left\| \mathbf{d}^{*}_{h2k2l2} \right\|}$$

All these relationships are widely used by the CaRIne software.

8.2 Menu *Specials/Reciprocal Lattice*

Using this menu, you will be able to create the reciprocal lattice, to change its spreading or to make a plane cut by selecting a zone axis.

Creation

This function creates a new window where the reciprocal lattice will be displayed. The title of this new window will correspond to the direct lattice from which it has been created.

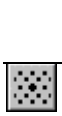
The reciprocal lattice follows the orientation of the real lattice (projections, rotations,…).

It is possible to copy the reciprocal lattice in the clipboard (WMF format, see Menu ***Edit***), to print or save the image on a disk (see Menu ***Files***).

The calculation of the reciprocal lattice takes into account the structure factors. In case of an extinction, the radius of the corresponding sphere is null, and the plane indices are not displayed.

Spread Of...

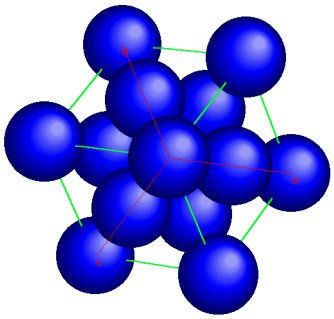
This function allows the spreading of the reciprocal lattice in the 3 directions (h, k and l). If you desire to cut the reciprocal lattice by a plane normal to the zone axis (the zone axis indices correspond to the current [uvw] direction), you will simply have to check the check box ☒ **Using zone axis** (see the following function).

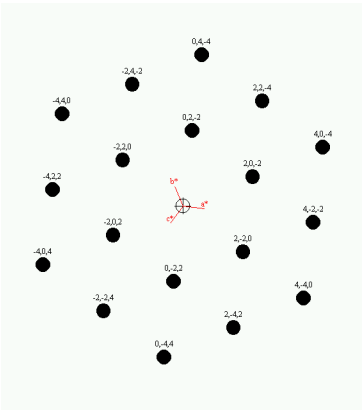


Zone Axis Ctrl-Z

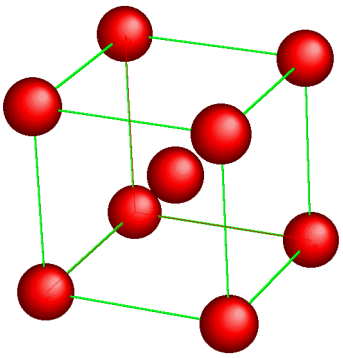
This function performs a plane cut of the reciprocal lattice. This cut is defined by a [uvw] zone axis. CaRIne will automatically make a projection following the zone axis direction. The defined zone axis becomes the current [uvw] direction (see Menu ***hkl/uvw***).
When activating this function, CaRIne will ask for a Delta S value. This value corresponds to the maximum distance (Å $^{-1}$) between the displayed nodes and the reciprocal plane perpendicular to the zone axis (see appendix B to set the default value of Delta S).

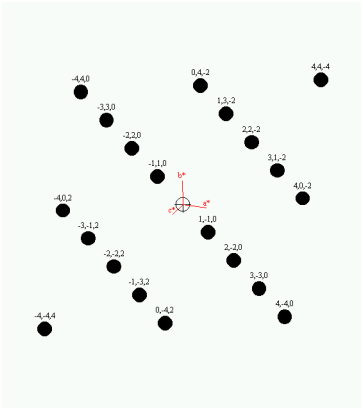
Examples :





Cut of the reciprocal lattice for the FCC Aluminium with a (111) zone axis.





Cut of the reciprocal lattice for the BCC Iron with a (112) zone axis.

? dhkl with mouse

This function gives the interplanar spacings of (hkl) planes just by selecting the corresponding node of the reciprocal lattice, with the mouse. This value is then inversely proportional to the distance between the selected node and the origin of the lattice.

? angle hkl with mouse

This function gives the angle between two planes, by selecting their nodes on the reciprocal lattice.

8.3 Menu *View*

This menu allows the selection of the graphical options.

Graphics Ctrl-G

As for the direct lattice, this function allows to select independently the objects to be displayed : nodes, indices, reference frame, links. It is also possible to activate/deactivate the perspective view.

General Scale Ctrl-E

This function acts on the size of all the reciprocal objects. The value of the scale is directly proportional to the object sizes (between 1 and 2000).

Note that this scale is independent from the real lattice scale. Nevertheless, proportions are respected. For example, if we increase the size of the real lattice by a factor 2, then the size of the reciprocal lattice objects will be decreased by a factor 2.

Radii Scale Ctrl-X

The size of the reciprocal lattice nodes can be modified independently from the other objects.

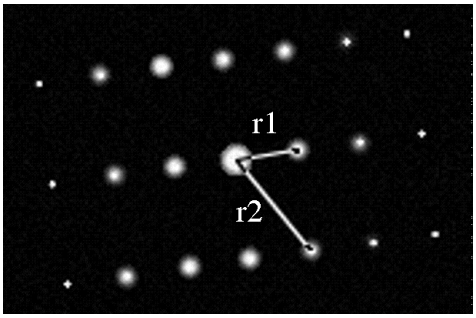
CHAPTER 9
CaRIne in examples

9

Follow these examples and exercises to get acquainted with the software logic and capabilities.

9.1 Indexing of a diffraction pattern

The following diffraction pattern (F9.1) has been obtained from a thin crystal of aluminium (FCC, a=4.049 Å) placed in an 100 kV electron microscope. The camera length corresponding to the print scale is 524 mm.



F9.1 : electron diffraction pattern (ZOLZ)

Question : Index the diffraction spots and determine the zone axis.

Solution :

1/ Without CaRIne

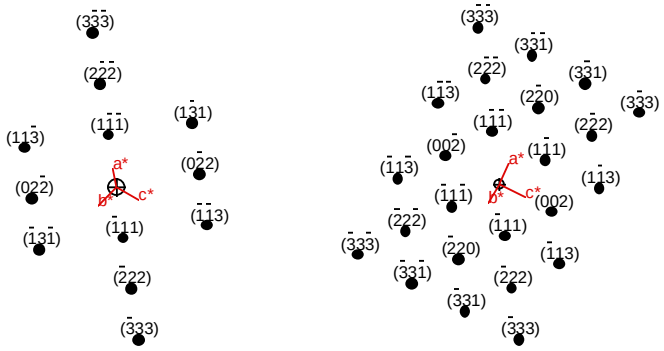
a/ take distances and angles on the diffraction pattern;
b/ determine the extinction conditions in the FCC lattice;
c/ make a list of the (hkl) planes with their interplanar spacings;
d/ compute the corresponding distances on the film;
e/ determine the different possibilities of indexing, check that the angles are correct, determine the zone axis.

2/ Using CaRIne

a/ take distances and angles on the diffraction pattern;
b/ load the aluminium FCC unit cell from the cell library (Menu ***Files***, function " **Load Cell**") or create this cell using the FCC Bravais' lattice. Check that a=4.049 Å;
c/ use the " **Identification of Planes** " function from the Menu ***Calcul*** :
- enter the accelerating voltage (100kV) and select the [>] button which will compute the corresponding wavelength (0.0388 Å);
- enter the camera length (52.4 cm) and select the [>] button which will give the camera constant (K=2.03 cm.Å);
- enter two distances, obtained from the diffraction pattern, with the angle between the two spots (for example, r1=0.85cm and r2=1.6cm and α= 58.5°). Click on [>] to compute the corresponding interplanar distances (you should get d1=2.39Å and d2=1.27Å);
- click on [Compute].

As a result of this sequence, CaRIne answers with a list of possibilities, ordered according to the increasing error between the computed solution and the experimental data. For the present example, the {111} - {311} solution with a [221] zone axis corresponds to a sum of errors (on d1, d2 and α) of 6.1%. The following solution {111} - {221} with a [110] zone axis, corresponding to a sum of errors of 14.9%.

Now, we just have to show these 2 solutions in order to choose between them. To do so, we need to create the reciprocal space (Menu ***Special*** / " **Reciprocal lattice** "-"**Create**"). To obtain the "3" indices, use the Menu ***Special*** / " **Reciprocal lattice** " - "**Spread of** "). Ask for the desired zone axis ([221] and [110]) using Menu ***Special*** / " **Reciprocal lattice** " - " **Zone axis** "). The figure F9.2 shows these results.



F9.2 : Plane cuts of the reciprocal lattice computed by CaRIne
a) left : zone axis [211] b/ right : zone axis [110].

Comparing the F9.2 with F9.1 clearly shows that the correct solution is [211]. The diffraction pattern is automatically indexed.

9.2 Standard projections of a cubic crystal

Question : Trace the standard projections (001) and (011) of a cubic crystal. Show the planes lying in a 100, 001, 110, 111 or 112 zone on a stereographic projection.

Solution :

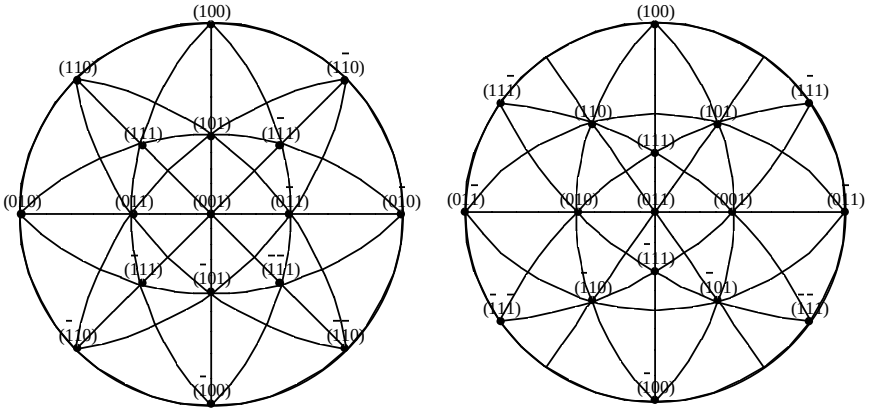
The sequence to follow is given below :

1/ Create a simple cubic lattice : a simple way to do so is to use Menu ***Cell*** / function "**Cubic** " - "**Simple**".

2/ Create a stereographic projection. You can either call the function "**Create**" from the Menu ***Specials/Stereo. Proj.*** , or click on the stereographic projection icon (below the rotation tools).

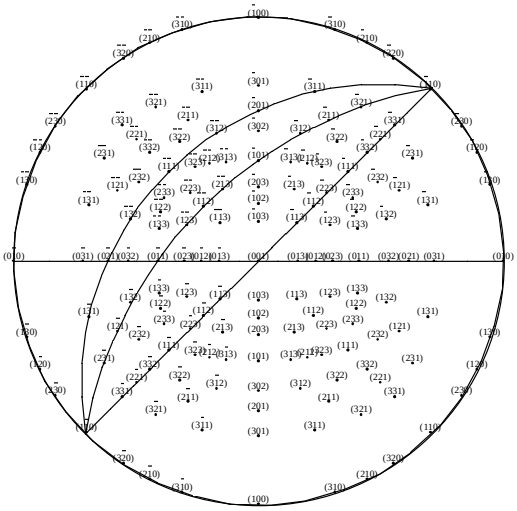
3/ Ask for the display of all indices between -1 and 1 : click on the stereographic projection window, outside of the circle. You can also use the function " **Parameters**" from the Menu ***Specials/Stereo. Proj.***. In the dialogue box, click on Pôles (and later on Traces) and give the indices ranges.

4/ Orient the stereographic projection : this can be done by using the Menu ***hkl/uvw*** function " **Proj. perp. plane** ", after having selected the plane #1 in the planes dialogue box (function " **Choice of hkl planes**" from the Menu ***hkl/uvw***). You will get the following figures :



F9.3 : Stereographic projection a) left : 001 b) right : 011.

To visualise the planes perpendicular to a specific plane, we can build a stereographic projection with all the poles with indices between -3 and +3. Then, we add the trace of the specific plane. The poles lying on the trace are the solutions (see F9.4).



F9.4 : 001 projections in the cubic system, of the poles with indices between -3 and +3, and the traces of planes (100), (001), (110), (111) and (112).

9.3 ABCABC… sequence in FCC and ABAB… sequence in HCP

Question : Show the sequence of compact planes in the FCC and HCP lattices.

Solutions :

a/ For the FCC structure, we want to show the construction of the lattice as a ABC stacking of {111} planes :

1• Open a new window (Menu ***File*** / function "**New**" or Ctrl-N).
2• Select a face-centred cubic lattice (Menu ***Cells*** / function "**Cubic/Face-Centred (F)**") and choose an atomic radius of 1Å with a lattice parameter of a=2.828Å in order to get a compact structure. It is not an obligation to select a chemical symbol and a level of oxidation for the element.
3• To work in several cells, expand the lattice using Menu ***Crystal*** / function "**Spread Of...**".
4• Select the (111) as the plane #1 in the plane dialogue box (Menu ***hkl/uvw*** / function "**Choice of hkl planes**").
5• Change the colour of all atoms belonging to a particular (111) plane : use the function "**Modify atom**" (Menu ***Crystal***, crystal tools, or Ctrl-M), click its colour and select ☒ **modify all atoms of the same plane**. This process will give you the "A" plane.
6• Translate this plane using the function " **Translation+plane n°1** " from the Menu ***hkl/uvw*** (or Ctrl-B).
7• Modify the colour of this plane as in number 5/. This will give you the "B" plane.
8• Repeat 6/ and 7/ to get the "C" plane.

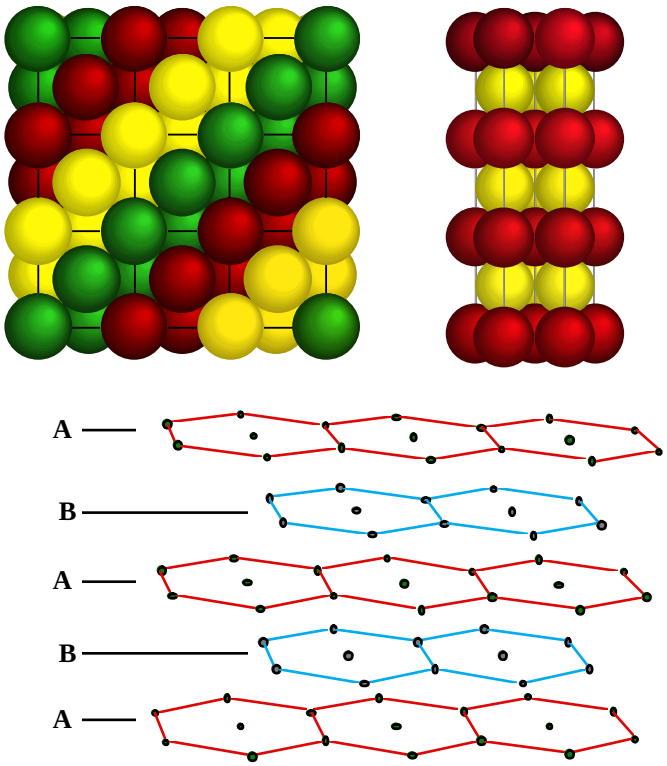
The resulting figure is given in figure F9.5.

b/ For the HCP lattice, we want to show the ABAB… stacking of the (001) planes :

Basically, you proceed as in ref a/. You use the HCP unit cell given in the Cells library. We can also use the hexagonal Bravais lattice, and we

place one atom in 0,0,0 and one in 1/3,2/3,1/2 using the function "**Creation**" / Menu ***Cell***. A third possibility is to use the space group (Menu ***Cells***) number 194 with one atom in 1/3,2/3,1/4. To obtain a compact structure, we set the parameter "a" to 2Å and the atomic radii to 1Å.

To obtain the figure F9.5, it is necessary to expand the unit cell in the **a**, **b** and **c** directions, and then to remove some atoms with the function "**Remove Atom**" / Menu ***Crystal*** (or using the corresponding Crystal tool). The last figure is obtained with a very small radii scale (function "**Radii Scale** " / Menu ***View***, or Ctrl-X). You then use the function "**Multilink**" (see Chap.2), after having differentiated the atoms to link with different colours. One can also add links one by one using the Crystal tool or the function "**Link**" / Menu ***Crystal*** .



F9.5: ABCABC… stacking in FCC (top left), ABAB… stacking in HCP (top right and bottom).

9.4 Visualisation of the (111) surface of diamond

Question : Visualise the (111) surface of the diamond structure.

Solutions :

First, you have to create a diamond crystal. To do so, we have several solutions :

1 - load the diamond cell from the cells library;
2 - create the diamond cell from the atomic positions (see §3.5);
3 - create the diamond cell from the space group (see §3.6).

The next step consists in expanding the crystal (function " **Spread of** " / Menu ***Crystal***) to 3*3*3 or 4*4*4 cells in order to better visualise the planes. The general scale (keys - et +) might need to be changed.

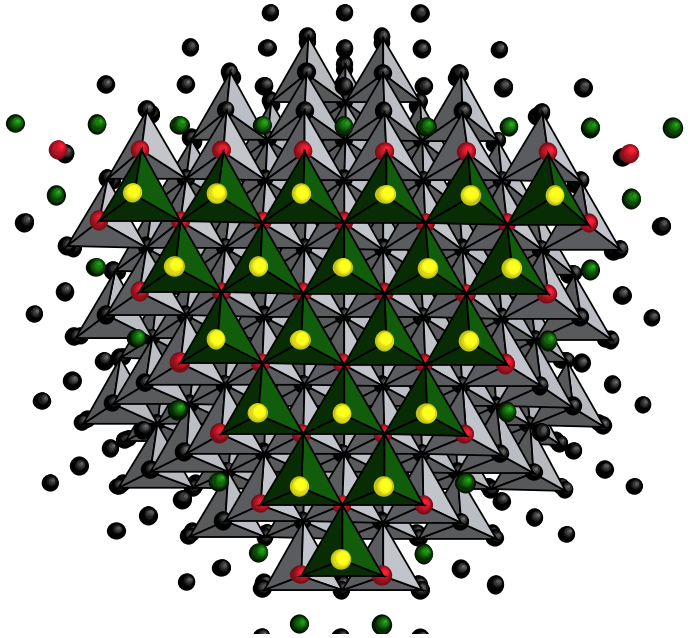
Then, you select the (111) plane (function " **Choice of hkl planes** " / Menu ***hkl/uvw***). If we give a "thickness" to this plane (E=0.1), we can see some atoms close to the (111) plane. To visualise this s tructure, you use a 20% radii of and you do a projection parallel to a direction belonging to the (111) plane ([01-1] for example) : function " **? [uvw] with mouse** ", click on two atoms of the (111) plane, and then select "**Projection // [uvw]**.

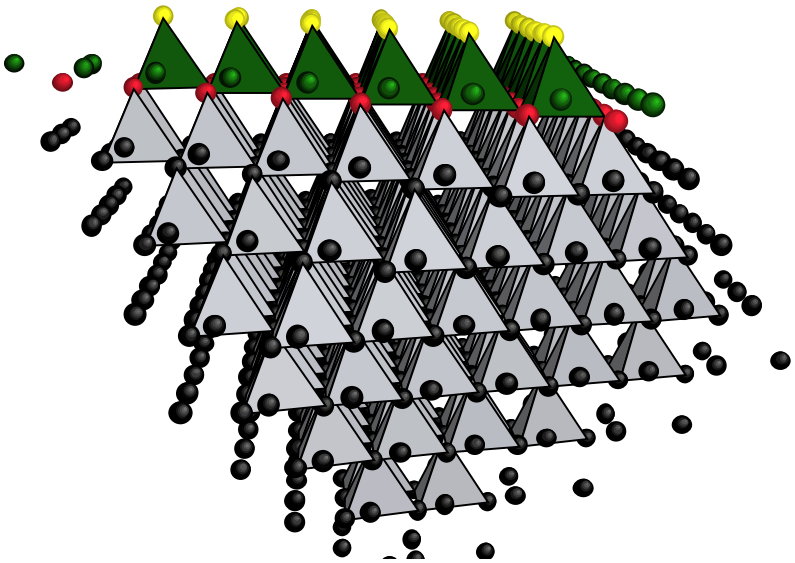
A nice way to visualise the different layers is to use different colours. We can also use the polyhedrons of coordination to show the diamond structure. We can follow the sequence given below :

1/ create the diamond lattice;
2/ using the " **Creation** " dialogue box / Menu ***Cells***, give a different colour to the interstitials
3/ expand the crystal;

4/ cut the crystal with a (111) plane, with E=0.1 (function " **Choice of hkl planes**"), make a projection // [01-1];
5/ translate this plane (function " **Translation + plane 1** ") to obtain a maximum of selected atoms;
6/ change the colour of all the atoms of this plane (function " **Modify Atom**");
7/ ask again for the (111) plane, but this time with E=0, and cross off the "cut option";
8/ translate this plane to superpose it to the one selected in 5/;
9/ give a new colour to this plane;
10/ destroy all hidden atoms (crystal tools);
11/ translate again (B);
12/ give a third colour;
13/ ask for the coordination polyhedrons from an atom located in the tetrahedral site.

Remark : the polyhedrons take the colour of their central atom.





F9.6 : Visualisation of the (111) plane of the diamond structure. Projection perpendicular to the (111) plane (previous page), and projection parallel to the [0 1 -1] direction.

9.5 X-Rays diffraction : Au-Cu alloys

Question : Compare the X-Rays diffraction patterns of the ordered AuCu alloy to the disordered AuCu alloy (50 at% Cu).

Data :	Gold (Au) :	FCC, a=4.08 Å
	Copper (Cu) :	FCC, a=3.61 Å
	Disordered AuCu alloy :	FCC, a=3.84 Å
	Ordered AuCu alloy :	tetragonal, a=3.98 Å and c=3.72 Å.

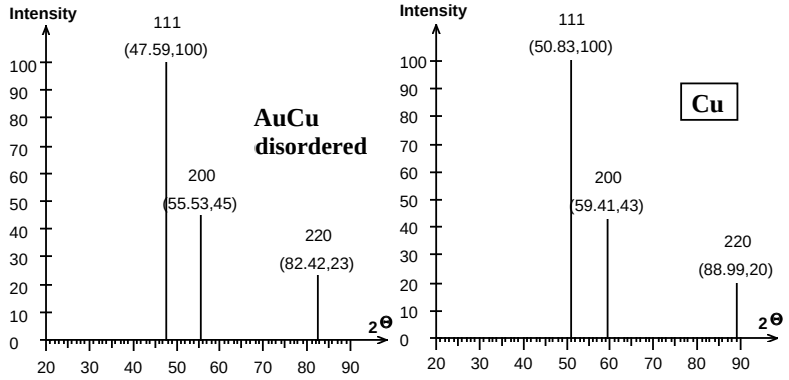
The last structure can be described as a Gold FCC cell, with a substitution of (002) plane Gold atoms by Copper atoms. This substitution leads to a slight contraction of the c-axis.

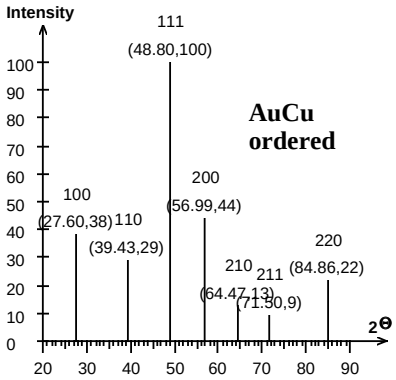
Solutions : The aim of this problem is to superpose the X-Ray diffraction diagrams of an ordered and disordered Au-Cu solid solutions of the same composition (50at% Au, 50at%Cu). We will then see additional peaks in the ordered structure. From the software user point of view, we will also learn how to share a same site between different kinds of atoms.

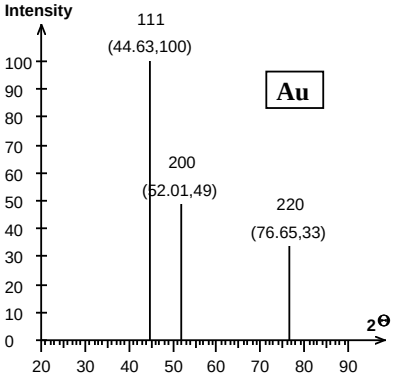
Creation of the unit cells : The Gold, Copper and disordered AuCu alloy are FCC cells. One solution is then to use the 225 th space group ($Fm\bar{3}m$) (function ***"Space Group"*** / Menu ***Cell***). For the Gold, we place an atom Au at 0,0,0 and we set the "a" parameter to 4,08Å. This cell is saved as "Au Gold Metal Cubic". For the Copper, we use a=3.61Å, and the cell is saved as "Cu Copper Metal Cubic". For the disordered alloy, the procedure is slightly different. We create two sites in 0,0,0. The first one is occupied by Au atoms, with an occupancy of 0.5. The second one is occupied by Cu atoms, with an occupancy of 0.5. This cell is saved under the name "Au Cu FCC disordered".
The ordered alloy can be built from the Gold FCC cell previously described. We then load the "Au Gold Metal Cubic" and save it with the new name "AuCu ordered (tetragonal)". In order to modify the a,b and c parameters, and in order to substitute Copper atoms to Gold atoms, we use the function "**Creation**" / Menu ***Cells***. Then, we save this again.

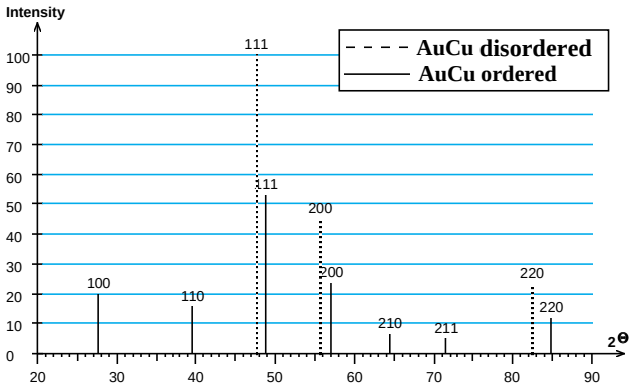
X-Rays diffraction diagrams : The first step is to load the two structures (ordered and disordered). Then, we need to associate them. To do so, we "active" the "AuCu FCC Disordered" window by clicking inside. Then we select the function "**Associated Lattices**" from the Menu ***Specials***. In the dialogue box which is then opened, we select "AuCu ordered (tetragonal)". Still from the "AuCu FCC disordered" window, we can now ask for the calculation of the X-Rays diffraction diagrams (function "**Create**", Menu ***Specials/RX***). Because the two lattices are associated, their diagrams will be superposed. It is possible (and recommended) to give a different pattern and colour to each diagram (see Chap.7). For the results presented in the following figure, we have used λ=0.1788965 nm (Kα1 Cobalt).

We can clearly observe the additional peaks for the ordered structure. We also observe a difference in the peaks positions due to the difference in cell dimensions.









Appendix A
Format Standard ASCII File and format of DOS versions files

This appendix describes the four file formats which allow CaRIne to exchange information with other software.

Remark : To get examples of these files, the best way is to build a cell or a crystal with CaRIne and to save it under one of these ASCII file formats.

A-1 "Cell Standard ASCII File"

This format is used to exchange the unit cell descriptions with other software. The files obey to the following structure :

CaRIne Crystallography 3.0	: Name of the application which has created the file.
Cell Standard ASCII File=Diamond.txt	: Name of the file.
File Version Number=1	:
Colors Referred to : Mendeleev Table	: Reference for the colour of atoms. Here, the colour of atoms are given by the Mendeleev table used by CaRIne.
---------- *Cell Definition* ----------	: Beginning of the description of the unit cell, or motifwith space group.
Cell Parameters (Å and °)	: Cell parameters in Angstrom (Å) and in degrees (°).
a=3.57 b=3.57 c=3.57	

alpha=90.00 beta=90.00 gamma=90.00

System=Cubic : Crystalline system (Cubic, Triclinic, Monoclinic, Orthorhombic, Trigonal, Tetragonal, Hexagonal).

Space Group Number =not used : Space group number (between 1and 230). "not used" signifies that the space group symmetries are not used to build the unit cell.

Number of Positions in Cell=8 : Number of positions in the unit cell (if Space Group Number=not used),or number of non-equivalent atoms of the motif (if Space Group Number≠0)

Atom	*Oxi.*	*X*	*Y*	*Z*	*R(Å)*	*Occ.*	Beginning of the position list
C	*Co*	*0*	*0*	*0*	*0.77*	*1.0000*	For each position, one can read :
C	*Co*	*1/2*	*0*	*1/2*	*0.77*	*1.0000*	•the chemical symbol
C	*Co*	*0*	*1/2*	*1/2*	*0.77*	*1.0000*	•the degree of oxidation
C	*Co*	*1/4*	*1/4*	*3/4*	*0.77*	*1.0000*	("Co" indicates covalent state)
C	*Co*	*1/2*	*1/2*	*0*	*0.77*	*1.0000*	•the reduced co-ordinates in the
C	*Co*	*1/4*	*3/4*	*1/4*	*0.77*	*1.0000*	(**a**,**b**,**c**) reference frame
C	*Co*	*3/4*	*1/4*	*1/4*	*0.77*	*1.0000*	•the atom/ion radius (in Å)
C	*Co*	*3/4*	*3/4*	*3/4*	*0.77*	*1.0000*	•the occupation factor

The different colour references

In the preceding example, the colours of the atoms were referred to the Mendeleev table used by CaRIne. There are two other possibilities : "RGB Components" and "16 Colours Palette".

• RGB Components :

In this case, there are three supplementary fields for each position : *Red*, *Green* and *Blue*. These three values should belong to the interval [0,65535].

Example :

Atom	*Oxi.*	*X*	*Y*	*Z*	*R(Å)*	*Occ.*	*Red*	*Green*	*Blue*
C	*Co*	*0*	*0*	*0*	*0.77*	*1.0000*	*15528*	*15528*	*15528*
C	*Co*	*1/2*	*0*	*1/2*	*0.77*	*1.0000*	*2000*	*2000*	*2000*
C	*Co*	*0*	*1/2*	*1/2*	*0.77*	*1.0000*	*15528*	*15528*	*15528*
C	*Co*	*1/4*	*1/4*	*3/4*	*0.77*	*1.0000*	*5369*	*5369*	*5369*
C	*Co*	*1/2*	*1/2*	*0*	*0.77*	*1.0000*	*255*	*35200*	*14695*
C	*Co*	*1/4*	*3/4*	*1/4*	*0.77*	*1.0000*	*36895*	*15698*	*2365*
C	*Co*	*3/4*	*1/4*	*1/4*	*0.77*	*1.0000*	*235*	*2369*	*14596*

C	*Co*	*3/4*	*3/4*	*3/4*	*0.77*	*1.0000*	*25698*	*1023*	*36952*

• 16 Colours Palette :

In this case, there is one supplementary field for each position : "Colour". This colour belongs to the following list :

•Black	•Red	•Gray	•Lightred
•Blue	•Magenta	•Lightblue	•Lightmagenta/Pink
•Green	•Brown	•Lightgreen	•Yellow
•Cyan	•Lightgray	•Lightcyan	•White

Unit cell described from the space group

If the "Space Group Number" is different than "not used", then the file may contain either :

• the list of all positions of the unit cell,
or • the list of only non-equivalent positions.

In order to differentiate these two possibilities, a key-sentence should be placed just after the space group number :

• *Only Non Equivalent Positions are listed* : for the motif case,
• *All Positions are listed* : for the unit cell case.

• "Only Non Equivalent Positions are listed" example:

Space Group Number= ***227***
Only Non Equivalent Positions are listed

*Number of Positions in Cell=****1***

Atom	*Oxi.*	*X*	*Y*	*Z*	*R(Å)*	*Occ.*
C	*Co*	*1/8*	*1/8*	*1/8*	*0.77*	*1.0000*

• "All Positions are listed" example:

Remark that in this case there is a supplementary field for each position. This field indicates if the position is "equivalent" or not ("Eq." or "NonEq.").

Space Group Number= ***227***
All Positions are listed

Number of Positions in Cell= ***8***

Atom	*Oxi.*	*X*	*Y*	*Z*	*R(Å)*	*Occ.*	
C	*Co*	*1/8*	*1/8*	*1/8*	*0.77*	*1.0000*	***NonEq.***
C	*Co*	*1/8*	*5/8*	*5/8*	*0.77*	*1.0000*	***Eq.***
C	*Co*	*5/8*	*1/8*	*5/8*	*0.77*	*1.0000*	***Eq.***
C	*Co*	*5/8*	*5/8*	*1/8*	*0.77*	*1.0000*	***Eq.***
C	*Co*	*7/8*	*7/8*	*7/8*	*0.77*	*1.0000*	***Eq.***
C	*Co*	*7/8*	*3/8*	*3/8*	*0.77*	*1.0000*	***Eq.***
C	*Co*	*3/8*	*7/8*	*3/8*	*0.77*	*1.0000*	***Eq.***
C	*Co*	*3/8*	*3/8*	*7/8*	*0.77*	*1.0000*	***Eq.***

A-2 The "Crystal Standard ASCII File"

This file format is used to exchange crystals files with other sofwares. This format includes the informations relative to the unit cell (see §A.1) and the informations concerning the crystal (spreading, point defects, links, cartesian atomic positions, ...) and the display (orientation, scales, background colour,...).

The first part of the file corresponds to the "Cell Standard ASCII File", then come the informations relative to the crystal :

CaRIne Crystallography 3.0	: Name of the application which has created the file.
Cell Standard ASCII File=Diamond.txt	: Name of the file.
File Version Number=1	:
Colours Referred to : Mendeleev Table	: Reference for the colour of atoms. Here, the colour of atoms are given by the Mendeleev table used by CaRIne.
----------	: Beginning of the description of the unit cell, or motifwith space group.
Cell Definition	

…
…
…

Crystal Definition				: Beginning of the crystal definition.

(a,b,c) Frame :				: Co-ordinates of the cell reference frame vectors (**a**,**b**,**c**) in the cartesian orthonormal reference frame R_r (see Chapter 4).
Origin	*x=0*	*y=0*	*z=0*	: Origin of the (**a**,**b**,**c**) reference frame
i	*x=90.000*	*y=0*	*z=0*	: Co-ordinates of the vector **a**
j	*x=-0.000*	*y=90.000*	*z=0*	: Co-ordinates of the vector **b**
k	*x=-0.000*	*y=-0.000*	*z=90.000*	: Co-ordinates of the vector **c**
(X,Y,Z) Frame :				: Co-ordinates of the cartesian orthonormal reference frame Rr given in the screen referenceframe Re (see Chapter 4). This defines theorientation of the crystal relatively to the screen.
Origin	*x=0*	*y=0*	*z=0*	: Origin of the (**x**,**y**,**z**) reference frame
i	*x=1.000*	*y=0*	*z=0*	: Vector **x**
j	*x=0*	*y=1.000*	*z=0*	: Vector **y**
k	*x=0*	*y=0*	*z=1.000*	: Vector **z**

Spread Of :		: Spreading of the crystal.
na=1 nb=1 nc=1		: Number of cells in each direction.
Build from origin		: Key-sentence indicating if the lattice is expanded from the unit cell origin ("Build from origin") or from the unit cell centre ("Build from centre").
Planes and Direction:(1,0,0), (-1,-1,1), (0,2,-3), [1,1,1]		: crystallographic plans and direction indices currently used by CaRIne.
General Scale=30.00		: General scale (between 1 and 2000).
Radii Scale=100.00		: Radii scale (in %, real number between 1 and 400).
Graphical Options :		: Description of the graphical options :
Perspective=	*TRUE*	: Perspective effect.
Show Planes=	*TRUE*	: Display of atoms belonging to the selected planes.
Show Frame=	*TRUE*	: Display of all links between atoms.
Show Atoms=	*TRUE*	: Display of the atoms.
Show Polyhedrons=	*TRUE*	: Display of the coordination polyhedrons.
Shading Effect=	*FALSE*	: Shading effect.

Number of Atoms in Crystal=14 : Number of atoms in the crystal (all atoms, displayed or not).

For each position one can read on a same line :

- the reference number of the atom/ion,
- its chemical symbol ("*" indicates an unknown chemical symbol),
- its degree of oxidation,
- its co-ordinates in the cell reference frame (**a**,**b**,**c**),
- its co-ordinates in the cartesian reference frame linked to the screen (**x**,**y**,**z**),
- its atomic radius,
- eventually, the RGB components (see A.1). Here, the colours are referenced to the Mendeleev table,
- a boolean indicating if there is a vacancy on this site,
- a boolean indicating if the atom/ion is hidden,
- a boolean indicating if the atom/ion belongs to the plane #1,
- a boolean indicating if the atom/ion belongs to the plane #2,
- a boolean indicating if the atom/ion belongs to the plane #3,

#	Atom	Oxi	i	j	k	X	Y	Z	R(Å)	Vacancy	Hidden	p 1	p 2	p 3
1	*		1	0	1	45.00000	-45.00000	45.00000	1.00	FALSE	FALSE	F	F	F
2	*		0	1	1	-45.00000	45.00000	45.00000	1.00	FALSE	FALSE	F	F	F
3	*		1	1	1	45.00000	45.00000	45.00000	1.00	FALSE	FALSE	F	F	F
4	*		0	0	1	-45.00000	-45.00000	45.00000	1.00	FALSE	FALSE	F	F	F
5	*		1/2	1/2	1	-0.00000	-0.00000	45.00000	1.00	FALSE	FALSE	F	F	F
6	*		1/2	0	1/2	0.00000	-45.00000	0	1.00	FALSE	FALSE	F	F	F
7	*		0	1/2	1/2	-45.00000	0.00000	0	1.00	FALSE	FALSE	F	F	F
8	*		1	1/2	1/2	45.00000	0.00000	0	1.00	FALSE	FALSE	F	F	F
9	*		1/2	1	1/2	-0.00000	45.00000	0	1.00	FALSE	FALSE	F	F	F
10	*		1/2	1/2	0	0.00000	0.00000	-45.00000	1.00	FALSE	FALSE	F	F	F
11	*		0	0	0	-45.00000	-45.00000	-45.00000	1.00	FALSE	FALSE	F	F	F
12	*		0	1	0	-45.00000	45.00000	-45.00000	1.00	FALSE	FALSE	F	F	F
13	*		1	1	0	45.00000	45.00000	-45.00000	1.00	FALSE	FALSE	F	F	F
14	*		1	0	0	45.00000	-45.00000	-45.00000	1.00	FALSE	FALSE	F	F	F

Number of Links in Crystal=12 : Number of links between atoms in this crystal.

Atom#1	Atom#2	Thickness	Colour
3	1	1	Black
2	4	1	Black
3	2	1	Black
1	4	1	Black
3	13	1	Black
2	12	1	Black
4	11	1	Black
1	14	1	Black
13	12	1	Black
12	11	1	Black
14	11	1	Black
13	14	1	Black

: Beginning of the list of links.

For each link, we find on the same line :

- the reference number of the first atom,
- the reference number of the second atom,
- the thickness of the link,
- the colour of the link.

The colour of a link can be chosen in the following list :

Black,White,Cyan,Magenta,Red,Green,Blue,Yellow

Note : this version (1) of the Crystal Standard ASCII File does not allow the coordination polyhedrons list to be exported or imported.

A-3 The "Cell DOS File Format"

This format is used by the versions of CaRIne for DOS (1.0 to 2.5) to describe the unit cells. The signification of each line is given below :

# line	*Signification*
1	a {Ångstrom}
2	b
3	c
4	alpha {radians}
5	beta
6	gamma
7	Number of atoms in the unit cell
Atome1 (1)	x {reduced co-ordinates of the atoms - between 0 and 1}
Atome1 (2)	y
Atome1 (3)	z
Atome1 (4)	radius {Ångstrom}
Atome1 (5)	colour {integer between 1 and 16}
…	*and so on for all the atoms of the cell...*

A-4 The "Crystal DOS File Format"

This format is used by the versions of CaRIne for DOS (2.1 to 2.5) to describe the crystals. The signification of each line is given below :

The first part of the file corresponds to the unit cell (see §A.3).

# line	*Signification*
1	a {Ångstrom}
2	b
3	c
4	alpha {radians}
5	beta
6	gamma
7	Number of atoms in the unit cell
Atome1 (1)	x {reduced co-ordinates of the atoms - between 0 and 1}
Atome1 (2)	y
Atome1 (3)	z
Atome1 (4)	radius {Ångstrom}
Atome1 (5)	colour {integer between 1 and 16, see table A.1}
…	*and so on for all the atoms of the cell...*

The file continues with the description of the crystal. The value of the variable X is equal to 7 plus 5 times the number of atoms in a unit cell.

# line	*Signification*
X+1	value of the general scale
X+2	value of the radii scale (in % of full size)
	a list of Boolean follows (1=true), corresponding to the state of graphic options
X+3	1 = only the atoms of the selected planes /0 = all atoms
X+4	1 = reference frame xyz
X+5	1 = reference frame abc
X+6	1 = frame (connections between atoms)
X+7	1 = atoms displayed
X+8	1 = direction [uvw]
X+9	1 = perspective effect
X+10	1 = rapid display
X+11	1 = transparency
X+12	1 = nice display
	description of the crystal
X+13	number of unit cells in the a direction (na)

X+14	number of unit cells in the b direction (nb)
X+15	number of unit cells in the c direction (nc)
	*description of the reference frame (**x**,**y**,**z**)*
X+16	x0 {co-ordinates of the reference frame origin}
X+17	y0
X+18	z0
X+19	xX {co-ordinates of the vector X}
X+20	yX
X+21	zX
…	*same thing for the two other unit vectors*
X+28	Description of the abc reference frame (similar to the xyz ref. frame)
…	
	description of the three selected planes
X+40	h
X+41	k
X+42	l
X+43	epsilon ("thickness"}
X+44	ix {co-ordinates of the translation vector between two successive (hkl) planes}
X+45	iy {in the unit cell reference frame}
X+46	iz
X+47	tx {co-ordinates of the translation vector between the (hkl) plane which is}
X+48	ty {the closest to the origin, and the current (hkl) plane}
X+49	tz
…	*same thing for the two other planes*
X+70	u {co-ordinates of the current [uvw] direction}
X+71	v
X+72	w
X+73	number of atoms in the crystal
	for each atom
X+74	x {co-ordinates in the (**x**,**y**,**z**) reference frame}
X+75	y
X+76	z
X+77	radius
X+78	colour {integer between 1 and 16, see table A.1}
X+79	i {co-ordinates in the (**a**,**b**,**c**) reference frame}
X+80	j
X+81	k
X+82	1 = this atom is displayed, 0 = this atom is hidden
X+83	1 = this atom belongs to the plane number 1
X+84	1 = this atom belongs to the plane number 2
X+85	1 = this atom belongs to the plane number 3
X+86	1 = vacancy
X+87	the number of the atom/ion

The following information concerns the existing connections between the different atoms. The value of Y is X + 73 + 14n, where n is the total number of atoms.

# line	***Signification***
Y Y+1 …	number of links N° N° {on a same line, identification numbers of the connected atoms} …

0	Black	4	Red	8	Gray	12	Lightred
1	Blue	5	Magenta	9	Lightblue	13	Lightmagenta/Pink
2	Green	6	Brown	10	Lightgreen	14	Yellow
3	Cyan	7	Lightgray	11	Lightcyan	15	White

Table A.1 : Value of the colour of the EGA palette

0	black	4	blue
1	white	5	lightblue
2	red	6	pink
3	green	7	yellow

Table A.2 : Value of "the 8 colour palette"

Appendix B
Setting the default values with the registry

B

This appendix describes all the initialization parameters recorded in the registry

Modification of the registry

Attention :

All the initialization parameters are recorded in the Windows 95 or NT 4.0 registry. A normal use of CaRIne does not imply to modify these data. Most of these parameters can be modified inside the application itself. CaRIne save the new parameters when closing. Registry modifications should be done only when the option is not available in CaRIne.

These parameters are recorded under the following key :

HKEY_CURRENT_USER\Software\CaRIne\3.1

To modify them, use the registry editor of Windows (Menu *Start/Run regedit*).

Details of the registry list

Values in darken lines should not be modified by users as they can prevent CaRIne to work correctly. When modifying the registry, respect the formats : number of values, «space» between characters, ...

HKEY_CURRENT_USER\Software\CaRIne\3.1\Crystal

Creation/List=34 123 497 354 85 135 197 263 326 376

Background Color=1

Default background color for a new crystal window (1 for white, 0 for black).

abc frame=0 18

Color of the abc reference frame and size of characters. Colors are selected from table *A.2*.

xyz frame=4 18

Color of the xyz reference frame and size of characters. Colors are selected from table *A.2*.

Dhkl list=0 5 0 5 0 5

h, k, and l ranges for creation of a list of planes used for the Dhkl list calculation (*Calcul | Plane spacing list*).

Angle hkl list=-3 3 -3 3 -3 3

h, k, and l ranges for the angle between planes list calculation (*Calcul | planes angle list*).

HKEY_CURRENT_USER\Software\CaRIne\3.1\Directories

CEL=C:\CaRIne 3.1\Cells
MTF=C:\CaRIne 3.1\MTF
ACE=C:\CaRIne 3.1\Cell Standard ASCII File (ACE)
CRY=C:\CaRIne 3.1\Crystals
RES=C:\CaRIne 3.1\RES
ACR=C:\CaRIne 3.1\Crystal Standard ASCII File (ACR)
XRD=C:\CaRIne 3.1\Import-Export
Personal=Personal directory

CaRIne's librairies directories. To be modified when running CaRIne (Menu *Files* | *Options*).

HKEY_CURRENT_USER\Software\CaRIne\3.1\Reciprocal lattice

delta s=0.020

Maximum reciprocal distance between a node and the reciprocal lattice plane when using the *Special* | *Reciprocal Lattice* | *Zone axis* function.

Spread=-2 2 -2 2 -2 2

Ranges for the reciprocal lattices (hmin hmax kmin kmax lmin lmax).

Background color=1

Default background color for the reciprocal lattice windows (1 : white, 0 : black).

Node color=0

Reciprocal lattice nodes' color (to be chosen in table *A.2*).

Frame color=3

Reciprocal lattice frame's color (to be chosen in table *A.2*).

*a*b*c* frame=2 18*

Color of the abc reference frame and size of characters. Colors are selected from table *A.2*.

HKEY_CURRENT_USER\Software\CaRIne\3.1\Settings

```
Language=English
Building pictures=2 200 1
Larger buttons=FALSE
```

These options are to be modified with the function *File* | *Options*.

HKEY_CURRENT_USER\Software\CaRIne\3.1\Stereographic projection

Radii=90

Stereographic projection radius size (in mm) (for the printing).

Direction=-1 1 -1 1 -1 1

Ranges of indices for the directions list creation in *Special* | *Stereographic projection* | *Parameters* (umin umax vmin vmax wmin wmax).

Pole=-1 1 -1 1 -1 1

Ranges of indices for the planes list creation in *Special* | *Stereographic projection* | *Parameters* (hmin hmax kmin kmax lmin lmax).

Plane=-1 1 -1 1 -1 1

Ranges of indices for the trace of planes list creation in *Special* | *Stereographic projection* | *Parameters* (hmin hmax kmin kmax lmin lmax).

HKEY_CURRENT_USER\Software\CaRIne\3.1\Tools

General=0 0
Crystal=0 0
StereoProj=0 0
Rotations=878 544
Demo=0 0

HKEY_CURRENT_USER\Software\CaRIne\3.1\X-Ray Diffraction

Domain=0 60

Calculation domain of Bragg's angle for the XRD diagrams (in °).

Temperature factor=1.0

Isotropic temperature factor B.

Step=0.1

Mini intensity=1.00

Minimum intensity for the peaks to be indexed.

Integral breadth=0.1

Integral width of the XRD peaks (to be modified with the function *View* | *Graphics*).

Don't show peaks as sticks=TRUE

To be modified with the function *View* | *Graphics.*

Show envelope for each diagram=TRUE

To be modified with the function *View* | *Graphics.*

Show sum=TRUE

To be modified with the function *View* | *Graphics.*

Sum style=4 3

Color and style of the XRD peaks sum lines (see table *A.2*).

Background Color=1

Defaults background color of XRD window (1 : white, 0 : black).

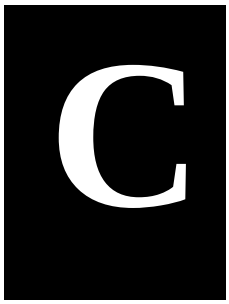
Grid color=2

XRD grid color (see table A.2).

Axis-Legend color=0

Default axis and legend colors for the XRD diagrams (see table *A.2*).

Appendix C
Diffusion factors for the atoms/ions

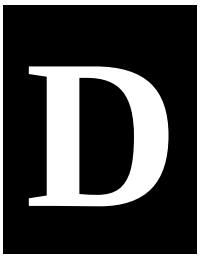


This is the list of atoms and ions differenciated by CaRIne when dealing with their diffusion factors as a fonction of sin θ/λ :

H	H^-	He	Li	Li^+	Be
Be^{2+}	B	C	C^{2+-}	N	O
O^-	F	F^-	Ne	Na	Na^+
Mg	Mg^{2+}	Al	Al^{3+}	Si	Si^{2+-}
Si^{4+}	P	S	Cl	Cl^-	Ar
K	K^+	Ca	Ca^{2+}	Sc	Sc^{3+}
Ti	Ti^{2+}	Ti^{3+}	Ti^{4+}	V	V^{2+}
V^{3+}	V^{5+}	Cr	Cr^{2+}	Cr^{3+}	Mn
Mn^{2+}	Mn^{3+}	Mn^{4+}	Fe	Fe^{2+}	Fe^{3+}
Co	Co^{2+}	Co^{3+}	Ni	Ni^{2+}	Ni^{3+}
Cu	Cu^+	Cu^{2+}	Zn	Zn^{2+}	Ga
Ga^{3+}	Ge	Ge^{4+}	Tb	Tb^{3+}	Dy
Dy^{3+}	Ho	Ho^{3+}	Er	Er^{3+}	Tm
Tm^{3+}	Yb	Yb^{2+}	Yb^{3+}	Lu	Lu^{3+}
Hf	Hf^{4+}	Ta	Ta^{5+}	W	W^{6+}
Re	Os	Os^{4+}	Ir	Ir^{3+}	Ir^{4+}
Pt	Pt^{2+}	Pt^{4+}	Au	Au^+	Au^{3+}
Hg	Hg^+	Hg^{2+}	Tl	Tl^+	Tl^{3+}
Pb	Pb^{2+}	Pb^{4+}	Bi	Bi^{3+}	Bi^{5+}
Po	At	Rn	Fr	Ra	Ra^{2+}
Ac	Ac^{3+}	Th	Th^{4+}	Pa	U
U^{3+}	U^{4+}	U^{6+}	Np	Np^{3+}	Np^{4+}
Np^{6+}	Pu	Pu^{3+}	Pu^{4+}	Pu^{6+}	Am
Cm	Bk	Cf	As	Se	Br
Br^-	Kr	Rb	Rb^+	Sr	Sr^{2+}
Y	Y^{3+}	Zr	Zr^{4+}	Nb	Nb^{3+}
Nb^{5+}	Mo	Mo^{3+}	Mo^{5+}	Mo^{6+}	Tc

Ru	Ru^{3+}	Ru^{4+}	Rh	Rh^{3+}	Rh^{4+}
Pd	Pd^{2+}	Pd^{4+}	Ag	Ag^{+}	Ag^{2+}
Cd	Cd^{2+}	In	In^{3+}	Sn	Sn^{2+}
Sn^{4+}	Sb	Sb^{3+}	Sb^{5+}	Te	I
I^{-}	Xe	Cs	Ba	Ba^{2+}	La
La^{3+}	Ce	Ce^{3+}	Ce^{4+}	Pr	Pr^{3+}
Pr^{4+}	Nd	Nd^{3+}	Pm	Pm^{3+}	Sm
Sm^{3+}	Eu	Eu^{2+}	Eu^{3+}	Gd	Gd^{3+}

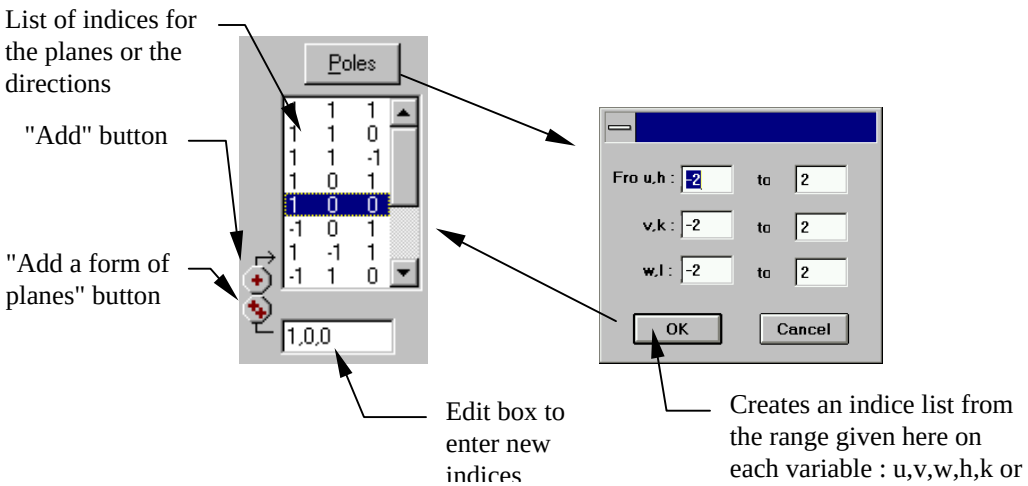
Appendix D
How to use the list generators



This appendix describes how to obtain a list of planes or directions using the list generators.

These generators can be found in the following functions :

- "**Planes spacing (list)**" of Menu ***Calcul***,
- "**Plans angle (list)**" of Menu ***Calcul***,
- "**Parameters**" of Menu ***Special/Stereo Proj***.


List of indices for the planes or the directions
"Add" button
"Add a form of planes" button
Poles
1 1
1 1 0
1 1 -1
1 0 1
1 0 0
-1 0 1
1 -1 1
-1 1 0
1,0,0
Edit box to enter new indices
Fro u,h : -2 to 2
v,k : -2 to 2
w,l : -2 to 2
OK
Cancel
Creates an indice list from the range given here on each variable : u,v,w,h,k or

A "list generator" is composed of :

- One button

to open the dialog box in which ranges are given.

- One field to enter new plane/direction one by one (values are separated with "," (commas)).

- One button to add the element corresponding to the previous field.

- One button to add a form of planes generated from the element corresponding to the previous field (only available for planes, not for directions).

- A context menu in order to : Remove all elements, Import/Export a list of elements from/to a text file. Click on the list box with the mouse (right button) to open this context menu :

- A list of all elements.

It is possible to move in a list with the keys : , . You can then select one element and delete it with the

(*del*) key of your keyboard (or double-click).

When a form of planes is generated, CaRIne opens a dialog box where planes can be selected or unselected before being added in the list of elements.

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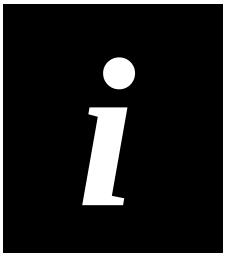

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